

# Thermo-Calc Documentation Set

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# Contents

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## **Quick Installation Guide: Windows® ..... 1**

Windows® Standalone Quick Install Guide ...	2
Request a License File .....	2
Install the Software .....	4
Step 1: Download and run your Thermo-Calc installation software .....	4
Step 2: Select the installation mode – typical or custom .....	5
Step 3: Customize your installation ....	5

## **Quick Installation Guide: Mac OS® . 1**

Mac OS® Standalone Quick Install Guide .....	2
Request a License File .....	2
Install the Software .....	4
Step 1: Download and install XQuartz .	4
Step 2: Download and run your Thermo-Calc installation software .....	4
Step 3: Select the installation mode ...	5

## **Installation Guide for all Platforms . 1**

Installing Thermo-Calc .....	2
System Requirements .....	3
Platforms Tested .....	3
Key to Using this Guide .....	3
License and Installation Types .....	7
License and Installation Types .....	8
About License Keys and Files .....	8
Standalone Installations (SUNLL) .....	8

---

Multi-User Network Installations (NWL) ....	9
Consolidated Network Installations ...	9
Distributed Network Installations .....	10
License Installations on a Server Network .....	10
Preparing for Installation .....	12
First Steps of Installation .....	13
Default Directory Locations .....	13
Subnet Information for Network Licenses .	16
Mac OS Installation Notes .....	17
Restarting After an Installation .....	17
Installing XQuartz .....	17
Enabling the Correct Security Settings	17
Linux Installation Notes .....	18
Installing Libgfortran .....	18
openSUSE Administration (sudo) Users	19
Opening Thermo-Calc in Linux .....	19
Standalone Installations .....	20
Typical Standalone Installations .....	21
Step 1: Request your license file from Thermo-Calc Software .....	21
Step 2: Download your Thermo-Calc installation software .....	21
Step 3: Run the applicable installation file for your operating system .....	21
Step 4: Select the installation type and upload the license file .....	22
Step 5: Install the software and start using Thermo-Calc .....	23

Add New Components to an Existing Installation .....	23	Installation Requirements .....	29
Custom Standalone Installation .....	23	Step 1: Stop any older versions of the License Server .....	30
Step 1: Complete Steps 1 to 4 of a typical standalone installation .....	23	Step 2: Write a script to start the License Server .....	30
Step 2: Select the installation type and what components to install .....	23	Step 3: Confirm the HOSTNAME variable and open the UDP port .....	31
Step 3: Set the installation directory path, license file location and shortcuts .....	24	Step 4: Start the License Server .....	31
Step 4: Install the software and start using Thermo-Calc .....	25	Thin Client Installations .....	31
Network Client Installations .....	26	Installation Requirements .....	32
Typical Network Client Installations .....	27	Custom Network Client Installations .....	33
Step 1: Install the licensing software .....	27	Step 1: Install the licensing software .....	33
Step 2: Complete Steps 1 to 4 of a typical standalone installation .....	27	Step 2: Complete Steps 1 to 4 of a typical standalone installation .....	33
Step 3: Choose the installation type and enter the computer server details .....	27	Step 3: Choose the installation type and what to install .....	33
Step 4: Install the software and components .....	27	Step 4: Set the installation directory path to the license file .....	34
Set Up the License Manager on Windows .....	28	Step 5: Specify the configuration and create shortcuts .....	35
Installation Requirements .....	28	Step 6: Install the software and start using Thermo-Calc .....	35
Step 1: Install the Sentinel RMS License Manager software .....	28	Unattended Network Client Installations .....	35
Step 2: Choose the installation directory .....	28	Step 1: Create an option file in a text editor to enter the options .....	35
Step 3: Choose the setup type and install the software .....	29	Step 2: Go to the directory where the installation file is stored .....	36
Step 4: Copy the license files to the destination directory .....	29	Request License Files .....	37
Set Up the License Server on Linux .....	29	Request a License File from Thermo-Calc Software .....	38
		Getting License Information Using Thermo-Calc .....	38



---

Requesting the License File for Windows ..	39
Requesting the License File for Mac OS ....	41
Requesting the License File for Linux .....	42
Troubleshooting .....	44
License Errors .....	45
Determining the Current License File Directory Path .....	46
From Thermo-Calc .....	46
Specifying a New Server Name or IP Number .....	49
Changing the server name or address (Windows) .....	50
Mac installations .....	50
Linux installations .....	50
MATLAB® Installation Directory .....	50
Firewalls .....	51
Client/Server Mismatch .....	51
Step 1: Compare computer names on the client computer and server ..	51
Step 2: Try these options to correct the issue .....	52
Mac OS Installations: Running the License Initialization Script .....	53
Linux Installations: Running the License Initialization Script .....	54
Uninstalling Thermo-Calc .....	56
Uninstalling Thermo-Calc .....	57
Uninstalling Standalone Versions of TC-PRISMA .....	59

## **Thermo-Calc User Guide ..... 1**

---

Introduction to Thermo-Calc .....	2
The Thermo-Calc Software .....	3
Typographical Conventions .....	3
Graphical Mode vs Console Mode .....	4
Switching Between Modes .....	5
Help Resources .....	5
Online and Context Help .....	5
Examples, Documentation and Materials ..	7
Graphical Mode Example Collection ...	9
Examples of Thermo-Calc Activities ....	11
Console Mode Example Collection .....	14
The Thermo-Calc Modules and Activities ..	20
Displaying Thermo-Calc License Information .....	23
Using This Guide .....	24
The Graphical Mode Interface .....	26
The GUI Layout .....	27
Project Activities and the Tree Structure ...	28
Activity Successor and Predecessor Nodes	28
Creating Activities and Successors .....	29
Graphical Mode Workflow .....	31
Main Menu and Toolbar .....	32
Saving and Opening Thermo-Calc Project Files .....	34
Project Activity Nodes .....	34
Project and Activity Menus .....	36
Moving Windows .....	38

Moving Nodes in the Tree and Using the Grid .....	39
Node Status Markers .....	40
Graphical Mode Projects .....	42
The Quick Start Wizard .....	43
Creating a Project with the Quick Start Wizard .....	43
Creating a Project from a Template .....	46
Cloning Activities and Trees .....	47
Performing Projects, Trees and Activities ..	49
Using the Scheduler .....	49
The Event Log .....	51
Graphical Mode Activities .....	53
System Definer .....	54
The System Definer Settings .....	54
Creating a System Definer Activity .....	59
Property Model Calculator .....	60
Property Model Calculator Workflow ..	61
Defining the Property Model Calculator .....	64
About the Uncertainty Calculations ...	64
Phase Transition Model .....	68
Driving Force Model .....	69
Interfacial Energy Model .....	70
Estimation of Coherent Interfacial Energy .....	70
Coarsening Model .....	70
Equilibrium Model .....	72
Equilibrium Calculator .....	72

Setting Equilibrium Calculator Conditions .....	73
Setting Conditions for Simplified Mode .....	74
Calculating with a Fixed Phase (Advanced Mode) .....	75
Calculating and Plotting Functions ....	76
Precipitation Calculator .....	78
Configuration Window .....	78
Conditions Tab Settings .....	79
Isothermal .....	81
Non-Isothermal .....	81
TTT-Diagram .....	81
Options Tab Settings .....	82
Growth Rate Model .....	83
Numerical Parameters .....	83
Plot Renderer .....	83
About Legend Styles .....	91
Adding and Editing Plot Labels .....	92
Label Formatting .....	93
Entering a Mixture of Plain Text and Equations .....	93
Rotation Angle and Show Anchor ...	94
Changing the Plot Properties .....	95
Saving Plots .....	95
Plotting Several Calculations in One Diagram .....	96
Adding Axes to a Diagram .....	97
Merging Plots into One Diagram .....	99

Table Renderer .....	101	Macro Files .....	124
Defining the Table Columns .....	103	Workspace Files .....	126
Experimental File Reader .....	104	Main Menu Commands .....	127
Binary Calculator .....	104	Defining a System in Console Mode .....	127
Ternary Calculator .....	106	Equilibrium Calculations .....	130
Scheil Calculator .....	108	About Equilibrium Calculations .....	131
Scheil Calculator Advanced Settings .....	110	Calculating an Equilibrium .....	133
The Console Mode Interface .....	111	Calculating an Equilibrium with a Fixed Phase .....	134
The Console Mode Layout .....	112	Calculating an Equilibrium with Sus- pended or Dormant Phases .....	134
Console Window .....	113	Property Diagrams .....	136
Editing the Default Console Directory .....	114	About Property Diagrams .....	137
Console Mode Results Window .....	116	Calculating and Plotting a Property Dia- gram .....	137
Event Log Window .....	116	Calculating a Property Diagram One Phase at a Time .....	139
Console Mode Workflow .....	117	Calculating Several Properties in the Same Diagram .....	139
Performing Calculations in Console Mode .....	118	Phase Diagrams .....	140
Using the Command Line Prompt .....	119	About Phase Diagrams .....	141
Available SYS Module Com- mands .....	119	Calculating and Plotting a Phase Diagram .....	141
Moving Between Modules and Sub- modules .....	119	Calculating a Quasi-Binary Phase Diagram .....	142
Entering Command Names or Abbre- viations .....	120	Calculating a Quasi-Ternary Phase Dia- gram .....	143
Specifying Parameters .....	121	Scheil Simulations .....	144
Wild Card Characters .....	122	About Scheil Simulations .....	145
Controlling Console Output .....	123	Simulating a Scheil-Solidification .....	146
Command History .....	123	Plotting Additional Scheil Simulation Dia- grams .....	148
Log, Macro and Workspace Files .....	123		
Log Files .....	124		

T0 Temperature Simulations .....	150
T0 Temperature Simulations .....	151
Making a T0 Temperature Simulation .....	151
Paraequilibrium .....	153
About Paraequilibrium .....	154
Calculating a Paraequilibrium .....	154
Potential Diagrams .....	157
About Potential Diagrams .....	158
Calculating a Potential Diagram .....	158
Calculating a Potential Diagram with Different Pressure .....	159
Aqueous Solutions .....	161
About Aqueous Solutions .....	162
Calculating a Pourbaix Diagram .....	163
Plotting Additional Aqueous Solution Diagrams .....	165
Stepping Calculations in an Aqueous Solution .....	167
Pourbaix Examples TCEX40, 40A to 40E, and TCEX53 .....	168
Console Mode TAB Module .....	174
Tabulation of Chemical Substances, Phases or Reactions .....	175
Tabulating a Reaction .....	176
Tabulating a Substance or Solution Phase at Fixed Composition .....	177
Console Mode POST Module .....	179
Console Mode Visualization .....	180
Plotting Diagrams .....	180

Modifying Diagrams .....	181
Saving Diagrams .....	183
Loading Saved Diagrams .....	183
About the Database Files .....	184
Encrypted vs Unencrypted Database Files .....	184
Database Installation Folder .....	184
Database Initialization File .....	184
User Database Files .....	184
About Cached Database Files (Graphical Mode only) .....	185
Editing the Database Initialization File or Unencrypted Database File .....	185
Best Practice Recommendations .....	186
Database Checker .....	186
Changing Global Settings .....	187
General .....	188
Graphical Mode - Default Units .....	189
Graphical Mode: Activities .....	190
Global Settings: System Definition (System Definer) .....	191
Creating a Database Package .....	192
Clearing a Database Package Message .....	193
Global Settings: Calculation (Equilibrium Calculator) .....	194
Global Settings: Precipitation (Precipitation Calculator) .....	196
Global Settings: Scheil (Scheil Calculator) .....	198

Global Settings: Tabulation (Table Renderer) .....	199	GET_DATA .....	15
Global Settings: Graphical and Console Mode-Plotting .....	200	LIST_DATABASE .....	16
Global Settings: Console Mode Default Appearance .....	203	LIST_SYSTEM .....	16
<b>Console Mode Command Reference . 1</b>		NEW_DIRECTORY_FILE .....	17
Introduction to the Command Reference ....	1	REJECT .....	17
About the Console Command Reference ..	2	RESTORE .....	18
File Types .....	2	SET_AUTO_APPEND_DATABASE .....	19
General Commands .....	3	SWITCH_DATABASE .....	20
BACK .....	4	EDIT_EXPERIMENTS Commands .....	22
EXIT .....	4	Running the EDIT_EXPERIMENTS Com- mand .....	23
GOTO_MODULE .....	4	COMPUTE_ALL_EQUILIBRIA .....	23
HELP (? and ??) .....	5	EXPERIMENT .....	24
HELP .....	5	EXPORT .....	26
INFORMATION .....	5	IMPORT .....	27
MACRO_FILE_OPEN .....	5	LABEL_DATA .....	28
SET_INTERACTIVE .....	8	LIST_ALL_EQUILIBRIA .....	28
BINARY_DIAGRAM Commands .....	9	MAKE_POP_FILE .....	28
BINARY_DIAGRAM Module .....	10	READ .....	29
DATABASE_RETRIEVAL Commands .....	11	RESTORE_ALL_WEIGHTS .....	29
AMEND_SELECTION .....	12	SAVE_WORKSPACES .....	30
APPEND_DATABASE .....	12	SET_ALTERNATE_CONDITION .....	30
DATABASE_INFORMATION .....	13	SET_WEIGHT .....	33
DEFINE_ELEMENTS .....	14	STORE_ALL_WEIGHTS .....	34
DEFINE_SPECIES .....	14	TRANSFER_START_VALUE .....	34
DEFINE_SYSTEM .....	15	Experimental Data Files .....	36
		Commands in the Experimental Data Files (*.POP, *.DOP) .....	37

---

TABLE_HEAD, TABLE_VALUES and TABLE_END .....	39
COMMENT .....	40
FLUSH_BUFFER .....	41
GIBBS_ENERGY_SYSTEM Commands .....	42
ADD_COMMENT .....	43
AMEND_ELEMENT_DATA .....	43
AMEND_PARAMETER .....	44
Solution Models in the GIBBS Module .....	46
AMEND_PHASE_DESCRIPTION .....	52
AMEND_SYMBOL .....	57
CHANGE_STATUS .....	59
ENTER_ELEMENT .....	60
About the ENTER_PARAMETER Command .....	61
Defining the Parameter .....	61
ENTER_PARAMETER .....	64
About the ENTER_PHASE Command .....	67
ENTER_PHASE .....	69
ENTER_SPECIES .....	71
ENTER_SYMBOL .....	72
LIST_CONSTITUENT .....	77
LIST_DATA .....	77
LIST_PARAMETER .....	78
LIST_PHASE_DATA .....	79
LIST_STATUS .....	80
LIST_SYMBOL .....	82
READ_GES_WORKSPACE .....	83
REINITIATE .....	83

---

SAVE_GES_WORKSPACE .....	84
SET_R_AND_P_NORM .....	85
PARROT Commands .....	86
AMEND_PARAMETER .....	88
AMEND_SYMBOL .....	90
COMPILE_EXPERIMENTS .....	92
CONTINUE_OPTIMIZATION .....	94
CREATE_NEW_STORE_FILE .....	94
EDIT_EXPERIMENTS .....	95
About the ENTER_PARAMETER Command .....	95
Defining the Parameter .....	95
ENTER_PARAMETER .....	99
LIST_ALL_VARIABLES .....	101
LIST_CONDITIONS .....	102
LIST_PARAMETER .....	102
LIST_PHASE_DATA (from GIBBS) .....	103
LIST_RESULT .....	104
LIST_STORE_FILE .....	108
LIST_SYMBOL_IN_GES .....	108
OPTIMIZE_VARIABLES .....	109
READ_PARROT_WORKSPACES .....	109
RECOVER_VARIABLES .....	110
REINITIATE .....	110
RESCALE_VARIABLES .....	110
SAVE_PARROT_WORKSPACES .....	111
SET_ALTERNATE_MODE .....	111
SET_EXTERNAL_PARAMETER .....	111

SET_FIX_VARIABLE .....	112	LIST_SYMBOLS .....	158
SET_OPTIMIZING_CONDITION .....	113	LOAD_INITIAL_EQUILIBRIUM .....	158
SET_OPTIMIZING_VARIABLE .....	114	MAP .....	158
SET_OUTPUT_LEVELS .....	115	POST .....	160
SET_SCALED_VARIABLE .....	115	READ_WORKSPACES .....	160
SET_STORE_FILE .....	116	RECOVER_START_VALUES .....	160
POLY_3 Commands .....	117	REINITIATE_MODULE .....	161
ADD_INITIAL_EQUILIBRIUM .....	119	SAVE_WORKSPACES .....	161
ADVANCED_OPTIONS Descriptions .....	120	SELECT_EQUILIBRIUM .....	162
ADVANCED_OPTIONS .....	125	SET_ALL_START_VALUES .....	162
AMEND_STORED_EQUILIBRIA .....	133	SET_AXIS_VARIABLE .....	164
CHANGE_STATUS .....	135	SET_CONDITION .....	165
COMPUTE_EQUILIBRIUM .....	139	SET_INPUT_AMOUNTS .....	168
COMPUTE_TRANSITION .....	141	SET_NUMERICAL_LIMITS .....	168
CREATE_NEW_EQUILIBRIUM .....	143	SET_REFERENCE_STATE .....	169
DEFINE_COMPONENTS .....	143	SET_START_CONSTITUTION .....	171
DEFINE_DIAGRAM .....	144	SET_START_VALUE .....	171
DEFINE_MATERIAL .....	147	SHOW_VALUE .....	172
DELETE_INITIAL_EQUILIBRIUM .....	151	STEP_WITH_OPTIONS .....	172
DELETE_SYMBOL .....	151	TABULATE .....	187
ENTER_SYMBOL .....	151	POST Commands .....	188
EVALUATE_FUNCTIONS .....	155	Using the POST Module .....	190
LIST_AXIS_VARIABLE .....	155	ADD_LABEL_TEXT .....	190
LIST_CONDITIONS .....	155	APPEND_EXPERIMENTAL_DATA .....	192
LIST_EQUILIBRIUM .....	156	CHANGE_LEGEND .....	193
LIST_INITIAL_EQUILIBRIA .....	157	DUMP_DIAGRAM .....	194
LIST_STATUS .....	157	ENTER_SYMBOL .....	195

---

FIND_LINE .....	198
LIST_DATA_TABLE .....	198
LIST_PLOT_SETTINGS .....	199
LIST_SYMBOLS .....	199
MAKE_EXPERIMENTAL_DATAFILE .....	199
MODIFY_LABEL_TEXT .....	200
PLOT_DIAGRAM .....	200
PRINT_DIAGRAM .....	201
QUICK_EXPERIMENTAL_PLOT .....	201
REINITIATE_PLOT_SETTINGS .....	202
RESTORE_PHASE_IN_PLOT .....	202
SELECT_PLOT .....	202
SET_AXIS_LENGTH .....	203
SET_AXIS_PLOT_STATUS .....	203
SET_AXIS_TEXT_STATUS .....	203
SET_AXIS_TYPE .....	204
SET_COLOR .....	204
SET_CORNER_TEXT .....	205
SET_DIAGRAM_AXIS .....	206
SET_DIAGRAM_TYPE .....	208
SET_FONT .....	209
SET_INTERACTIVE_MODE .....	209
SET_LABEL_CURVE_OPTION .....	209
SET_PLOT_FORMAT .....	210
SET_PLOT_OPTIONS .....	211
SET_PLOT_SIZE .....	212
SET_PREFIX_SCALING .....	213

---

SET_RASTER_STATUS .....	213
SET_REFERENCE_STATE .....	213
SET_SCALING_STATUS .....	214
SET_TIC_TYPE .....	215
SET_TIELINE_STATUS .....	215
SET_TITLE .....	215
SET_TRUE_MANUAL_SCALING .....	216
SUSPEND_PHASE_IN_PLOT .....	216
TABULATE .....	216
POTENTIAL_DIAGRAM Module .....	217
POTENTIAL_DIAGRAM .....	218
POURBAIX_DIAGRAM Commands .....	219
POURBAIX_DIAGRAM Commands .....	220
Pause Options .....	222
REACTOR_SIMULATOR_3 Commands .....	228
CREATE_DIVIDERS .....	229
CREATE_PIPES .....	229
CREATE_STAGE_BOXES .....	230
EXECUTE_POLY3_COMMAND .....	231
LIST_RECORDS .....	231
READ_WORKSPACE .....	232
SAVE_WORKSPACE .....	232
START_SIMULATION .....	233
SCHEIL Commands .....	235
BCC_TO_FCC_TRANSFORMATION .....	236
EVALUATE_SEGREGATION_PROFILE .....	236
GLOBAL_MINIMIZATION .....	236



LIQUID_PHASE_NAME .....	236	TABULATE_REACTION .....	258
SAVE_FILE_NAME .....	237	TABULATE_SUBSTANCE .....	260
START_WIZARD .....	237	TERNARY_DIAGRAM Commands .....	267
TEMPERATURE_STEP .....	238	TERNARY_DIAGRAM Module .....	268
TERMINATION_CRITERIA .....	238	Thermodynamic Variables and Units .....	269
SYSTEM_UTILITIES Commands .....	239	Thermodynamic Variables .....	270
ABOUT .....	240	Common Thermodynamic Variables .....	270
CLOSE_FILE .....	240	How to Read the Tables .....	270
DISPLAY_LICENSE_INFO .....	240	Intensive Variables .....	271
HP_CALCULATOR .....	240	Extensive Variables .....	272
OPEN_FILE .....	241	Special Quantities .....	275
SET_COMMAND_UNITS .....	241	The u-Fraction Variable .....	276
SET_ECHO .....	242	Suffixes .....	276
SET_INTERACTIVE_MODE .....	242	Normalizing Suffixes .....	276
SET_LOG_FILE .....	242	Derived Variables and Partial Derivatives .....	281
SET_PLOT_ENVIRONMENT .....	243	Defining New Derived Variables and Functions .....	283
SET_TC_OPTIONS .....	243	Derived Variables for Aqueous Solutions .....	283
STOP_ON_ERROR .....	244	Defining New Derived Variables for Aqueous Solutions .....	287
TABULATION_REACTION Commands .....	245	Thermodynamic Variables and Wild-card Characters .....	287
ENTER_FUNCTION .....	246	Units of State Variables and Derived Variables .....	288
ENTER_REACTION .....	247	User-Specified Units .....	288
LIST_SUBSTANCES .....	249	Examples of User-Defined Units .....	289
SET_ENERGY_UNIT .....	251	For intensive variables of a defined system .....	289
SET_PLOT_FORMAT .....	251		
SWITCH_DATABASE .....	251		
TABULATE .....	253		
TABULATE_DERIVATIVES .....	253		

For extensive variables of a defined system .....	290	Entering Experimental Information .....	16
For intensive variables of a system component .....	290	Creating a New Equilibrium .....	16
For extensive variables of a system component .....	291	Setting Equilibrium Conditions and its Uncertainty .....	17
For intensive variables of a species in a phase .....	293	Setting Reference States .....	18
For extensive variables of a species in a phase .....	293	Entering the Experimental Value and its Uncertainty .....	18
<b>Data Optimization User Guide .....</b>	<b>1</b>	Entering Many Equilibria as a Table ....	19
Introduction .....	2	Setting Site Fraction Start Values .....	20
Introduction to Data Optimization .....	3	Commenting About an Equilibrium ....	21
Data Optimization .....	3	Simultaneous Use of Binary and Ternary Experiments .....	21
The Least-Squares Method .....	4	Using Stability Conditions .....	22
The CALPHAD Approach .....	4	Grouping Equilibria with Labels .....	22
Working with Data Optimization in Thermo-Calc .....	6	Dividing the POP-File into Several Blocks .....	22
Data Optimization in Thermo-Calc .....	7	The Setup File .....	24
Data Optimization Workflow .....	7	Creating the Setup File .....	25
The PARROT Module .....	8	Defining the System .....	25
The EDIT_EXPERIMENTS Module .....	8	Creating Additional Composition Sets of a Phase .....	26
Data Optimization in Other Modules .....	9	Entering the Optimizing Variables .....	26
Optimization File Types .....	9	Entering Optimizing Variables in Parameter Specifications .....	26
Optimization Workspaces .....	10	Entering Interaction Parameters .....	27
Method for Optimization and Simulation ..	10	Initializing Optimizing Variables in PARROT	28
Creating the POP-File .....	12	Creating the Workspace File .....	29
Experimental Information .....	13	Compiling the POP-file .....	29
POP-File Syntax .....	14	Returning Control to the Console .....	29

Optimizing in PARROT .....	30	Entering Other Experiments in the POP with Alternate Mode .....	45
Optimizing the System in PARROT .....	31	Troubleshooting .....	47
Changes that Require POP-file Recom- pilation .....	31	Useful Guidelines .....	48
Optimization Workflow .....	31	Excluding and Including the Correct Equi- libria .....	49
Ensuring Computation of all Equilibria .....	32	Conflicting Data .....	49
Setting Weights .....	33	Experiments and Experimental Data .....	50
Optimizing and Evaluating Results .....	34	Phase Diagram Data .....	51
The Critical Set of Experiments .....	34	Data for Individual Compounds .....	52
Continuing the Optimization and Resetting Variables .....	35	Single Phase Mixing Enthalpies or Partial Enthalpies .....	53
Updating the Set of Optimizing Variables .....	36	Enthalpies of Formation and Enthalpies of Reactions .....	54
Reducing the Number of Optimizing Vari- ables .....	38	Chemical Potentials via EMF Meas- urements .....	55
Plotting Intermediate Results .....	38	Driving Force for Metastable Phases .....	55
Superimposing Experimental Data from EXP-files .....	38	Pressure-Temperature-Volume EOS Data .....	56
Finalizing the Optimization .....	39	Crystal Structure, Lattice Parameters and Site-Occupancy .....	56
Finishing the Optimization .....	40	Magnetism and Other Atomistic Prop- erties .....	57
Rounding off Optimizing Variable Values .....	40	Data About Systems of Different Orders .....	58
Updating the Database File .....	40	Thermodynamic Models .....	59
Creating a Database File .....	41	Gas .....	60
Updating the Setup File and the POP-file .....	41	Compound Energy Formalism .....	60
Alternate Mode .....	42	Substitutional Liquid .....	60
About Alternate Mode .....	43	Ionic Two-Sublattice Liquid Model .....	61
Optimizing in Alternate Mode .....	43	Models for Ordered Phases .....	61
Preparing the POP-file for Alternate Mode .....	44	4SL Model for FCC, HCP and BCC .....	62
Examples of SET_ALTERNATE_CONDITION .....	44		

2SL Model for FCC, HCP and BCC .....	63	Size Distribution (PSD) Ni-8Al-8Cr .	18
Magnetic Ordering .....	64	Size Distribution (PSD) Ni-10Al-10Cr .....	19
Molar Volumes and High Pressure .....	64	<b>Console Mode Examples Guide .....</b>	<b>1</b>
Excess Models .....	65	About the Console Mode Examples Guide ...	2
<b>Graphical Mode Examples Guide .....</b>	<b>1</b>	Thermo-Calc-Console-Examples .....	4
About the Graphical Mode Examples .....	2	<b>Pourbaix Diagrams .....</b>	<b>1</b>
Examples of Thermo-Calc Activities .....	3	Introduction to Pourbaix Diagrams .....	2
Precipitation Calculator Examples .....	7	About Pourbaix Diagrams in Thermo-Calc .	3
Example 13: Isothermal Precipitation of Al <sub>3</sub> Sc .....	7	Pourbaix Diagrams .....	3
Plot Results .....	8	Working with Pourbaix Diagrams .....	5
Example 14: Stable and Metastable Carbides - Isothermal .....	9	Key Concepts .....	5
Plot Results .....	10	Effective Interaction Ratio .....	5
Example 15: Stable and Metastable Carbides - TTT Diagram .....	10	Solubility .....	6
Plot Results .....	11	Basic Settings and Definitions .....	7
Example 16: Precipitation of Iron Carbon Cementite .....	12	Thermodynamic Data Requirements .....	9
Volume Fraction .....	13	Required Thermodynamic Data .....	10
Example 17: Precipitation of g' in Ni Superalloys - Isothermal .....	13	Including or Excluding the Gas Phase .....	10
Volume Fraction .....	14	Examples of Pourbaix Diagrams for Fe .....	15
Number Density .....	15	Pourbaix Diagrams with Gas Phase Excluded .....	16
Mean Radius .....	15	Pourbaix Diagrams with Gas Phase Included .....	16
Example 18: Precipitation of g' in Ni Superalloys - Non-isothermal .....	16	Other Examples of Pourbaix Diagrams .....	18
Mean Radius Ni-8Al-8Cr .....	17	Variations of Pourbaix Diagrams .....	19
Mean Radius Ni-10Al-10CR .....	18	Pourbaix Diagrams for Complex Alloys .....	21
		Pourbaix Diagram References .....	23
		<b>DATAPLOT User Guide .....</b>	<b>1</b>

Introduction to the DATAPLOT User Guide ..	2	YTYPE .....	16
Using this Guide .....	3	XLENGTH .....	16
About the DATAPLOT Graphical Language ..	3	YLENGTH .....	16
DATAPLOT Examples .....	3	TIC_TYPE .....	16
Using DATAPLOT Graphical Language .....	4	TITLE .....	16
DATAPLOT File Structure .....	5	DIAGRAM_TYPE .....	17
DATAPLOT Language Syntax .....	5	DATASET Commands .....	18
Coordinate Systems .....	5	DATASET .....	19
Graphical Operation Codes .....	6	BLOCK .....	19
Tables or Blocks .....	7	BLOCKEND .....	20
Drawing a Polygon .....	8	DATAPOINT .....	20
Drawing an Analytical Function .....	8	CLIP .....	20
Painting of an Enclosed Area .....	8	ATTRIBUTE .....	20
Writing a Text .....	8	LINETYPE .....	21
Plotting a Symbol .....	9	DRAWLINE .....	21
Other Commands .....	10	CHARSIZE .....	22
Interactive Plotting .....	11	SYMBOLSIZE .....	22
Formatting DIGLAB Symbols in LaTeX Documents .....	11	GLOBALSIZE .....	22
LaTeX Formatting Codes .....	12	COLOR .....	22
LTEXT vs LaTeX Commands for Labels ..	13	FONT .....	24
PROLOGUE Commands .....	14	STRING .....	25
PROLOGUE .....	15	TEXT .....	27
XSCALE .....	15	FUNCTION .....	27
YSCALE .....	15	PCFUNCTION .....	27
XTEXT .....	15	PAINT .....	27
YTEXT .....	15	INCLUDE .....	28
XTYPE .....	15	Examples of DATAPLOT Files and Outputs ...	29

Example 1 – Draw Lines and Symbols .....	30	ALLOTROPIC_PHASE .....	16
Example 2 – Draw Polygons and Symbols ..	31	TEMPERATURE_LIMITS .....	16
Example 3 – Using Strings and Various Line Types .....	32	DEFINE_SYSTEM_DEFAULT .....	16
Example 4 – Draw Curves Defined by Func- tions .....	33	DEFAULT_COMMAND .....	17
Example 5 – Use Included Files for Pre- defined Symbols .....	34	DATABASE_INFORMATION .....	18
Example 6 – Plot Triangular Diagrams for Ternary Systems .....	37	TYPE_DEFINITION .....	18
Example 7 – Color Codes and Effects .....	41	FTP_FILE .....	21
<b>Database Manager User Guide .....</b>	<b>1</b>	FUNCTION .....	22
Introduction to the Database Manager Guide .....	2	PARAMETER .....	24
Thermodynamic and Kinetic/Mobility Data- bases .....	3	GIBBS Parameter Name .....	26
Initialization of the DATA Module .....	3	OPTIONS .....	31
Initiation Parameter Examples .....	4	TABLE .....	32
The Database Definition File and Keywords ..	6	ASSESSED_SYSTEMS .....	32
Database Definition File Syntax .....	7	REFERENCE_FILE .....	35
ELEMENT .....	7	LIST_OF_REFERENCE .....	36
SPECIES .....	8	ADD_REFERENCE .....	37
PHASE .....	9	CASE and ENDCASE .....	38
Examples of Recommended Suffixes ..	10	VERSION_DATA .....	39
GIBBS Phase-type Codes .....	10	Working with the Mobility Databases .....	40
Additional Clarification .....	11	About the Diffusion Module (DICTRA) and the Databases .....	41
CONSTITUENT .....	14	Extensions to Database Definition File Syn- tax .....	42
ADD_CONSTITUENT .....	15	PARAMETER .....	42
COMPOUND_PHASE .....	16	DIFFUSION .....	43
		ZERO_VOLUME_SPECIES .....	43
		Database Definition File Examples .....	44
		Example 1: A Steel Database .....	45

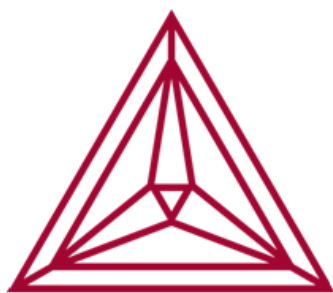
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Example 2: A Custom Database for the Sb-Sn Binary System .....	46
Example 3: A Public Database for the Fe-Cr-C Ternary System .....	49
The Database Checker .....	64
About the Database Checker .....	65
Database Checker Revision History .....	65
<b>Index .....</b>	<b>1</b>

# **Quick Installation Guide: Windows®**

**Standalone Operating Systems**

**Version 2016a**





## Windows® Standalone Quick Install Guide

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

**This guide is applicable to:**

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



Also see [License and Installation Types](#) on page 8 for detailed instructions for other operating systems and network installations.

### Request a License File

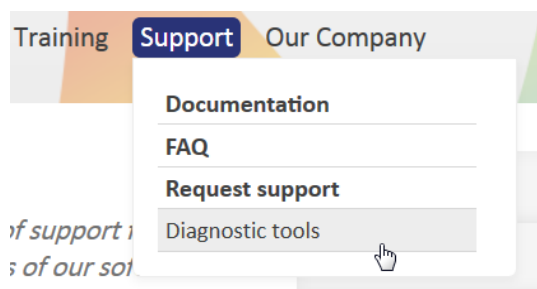


**Demo (trial) installations:** Skip this section. A license file is automatically installed with the software. You do not need to request it.

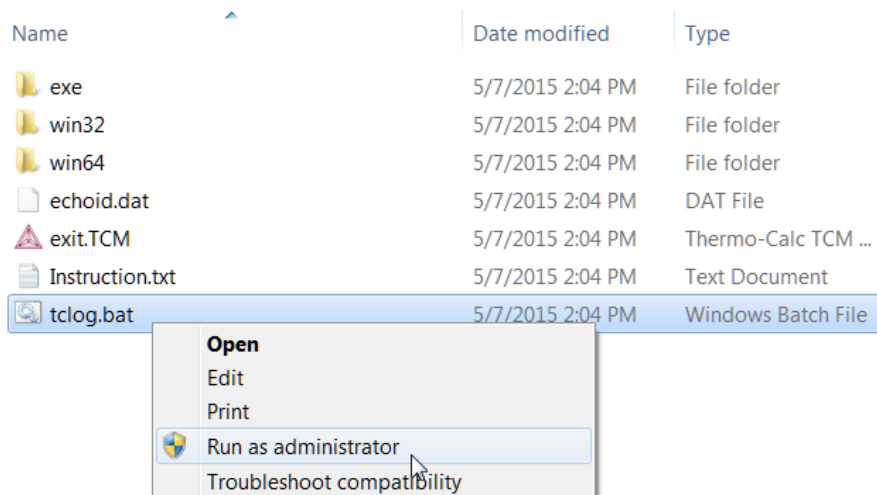


**Upgrades to a new version of Thermo-Calc:** Skip this section if you are upgrading to a new version of Thermo-Calc and (and you have a maintenance plan). Your license is sent to you in an email from Thermo-Calc Software AB. Save it to your computer to use during software installation.

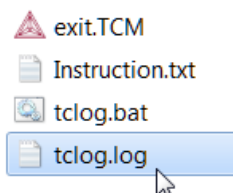
1. Go to Thermo-Calc's [website](#) (or click the link sent by email).



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



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



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

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


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



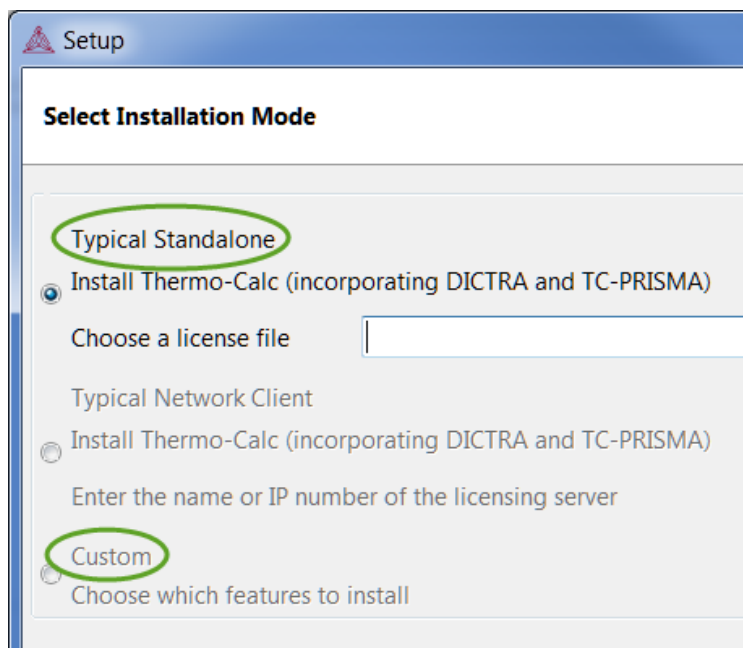
8. A representative from Thermo-Calc Software replies to the email and attaches your license file(s).
9. Save the license file(s) to your computer or network.

## *Install the Software*

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

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


## Step 2: Select the installation mode – typical or custom



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



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

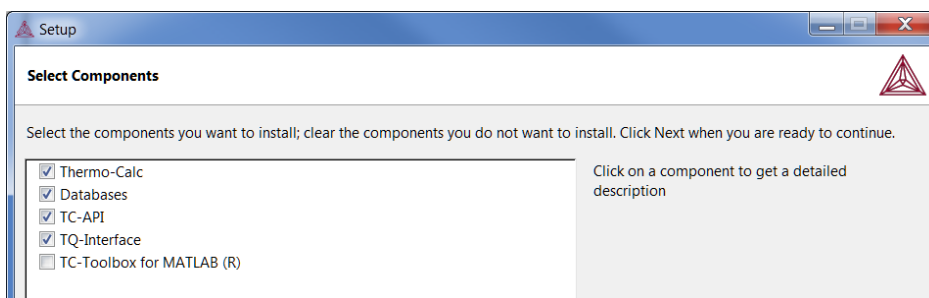
2. For a **Typical Standalone** installation, in the **Choose a license file** field click the file button  to navigate to where you saved the license file emailed to you from Thermo-Calc Software. The license file is called **lservrc**. Click **Next**.




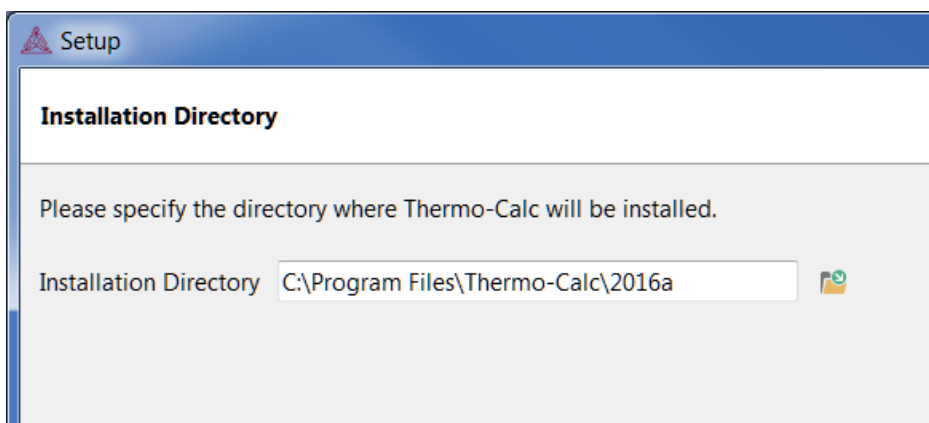
**DEMO Typical Standalone installations:** Your installation starts and is done when the **Completing the Thermo-Calc Demo Setup Wizard** opens. Click **Finish** and reboot your computer to start using Thermo-Calc.


## Step 3: Customize your installation

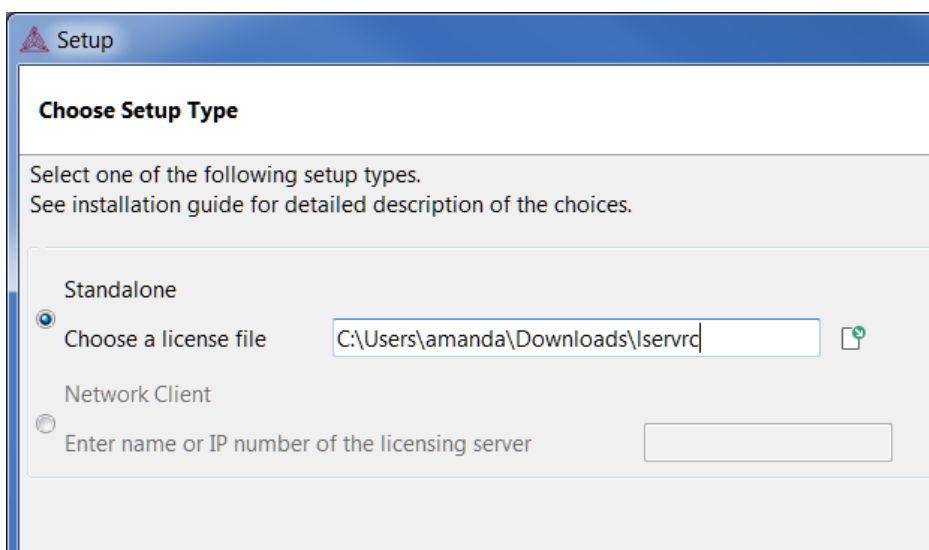
1. In the **Select Components** window, click to select what you want to install. Click **Next**.



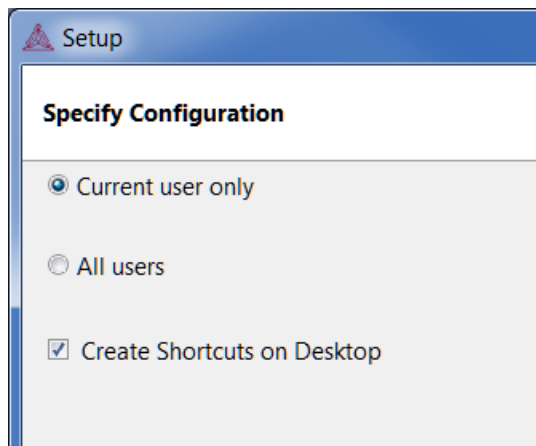
2. In the **Installation Directory** window, either accept the default, enter a file path or click the file button  to navigate to another directory.



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



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

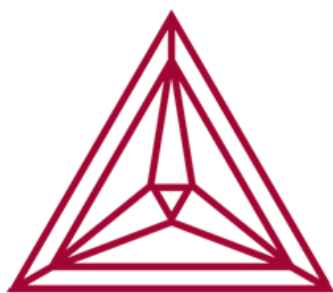


5. In the **Ready to Install** window click **Next**. Click **Finish** and start using Thermo-Calc.

# **Quick Installation Guide: Mac OS®**

**Standalone Operating Systems**

**Version 2016a**



## Mac OS® Standalone Quick Install Guide

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

**This guide is applicable to:**

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



Also see [License and Installation Types](#) on page 8 for detailed instructions for other operating systems and network installations.

### Request a License File



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



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

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

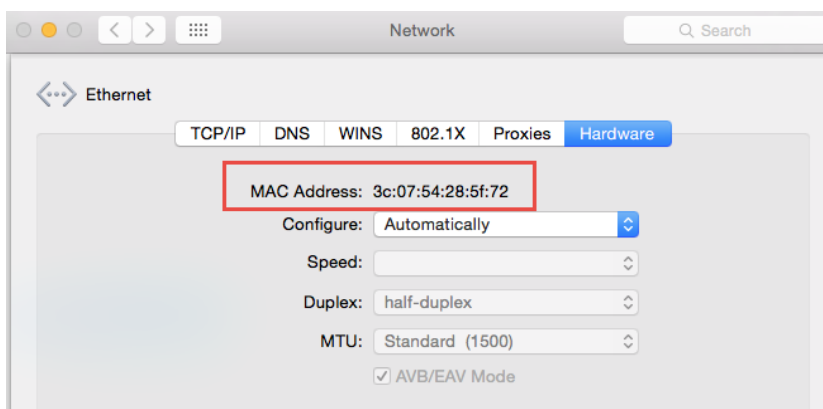




3. In the left column select **Ethernet** or **Built-in Ethernet** (do not select a WiFi connection as a local static MAC address is required).

4. Click **Advanced** → **Hardware**.

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



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

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

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

---



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

## ***Install the Software***

### **Step 1: Download and install XQuartz**

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

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

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

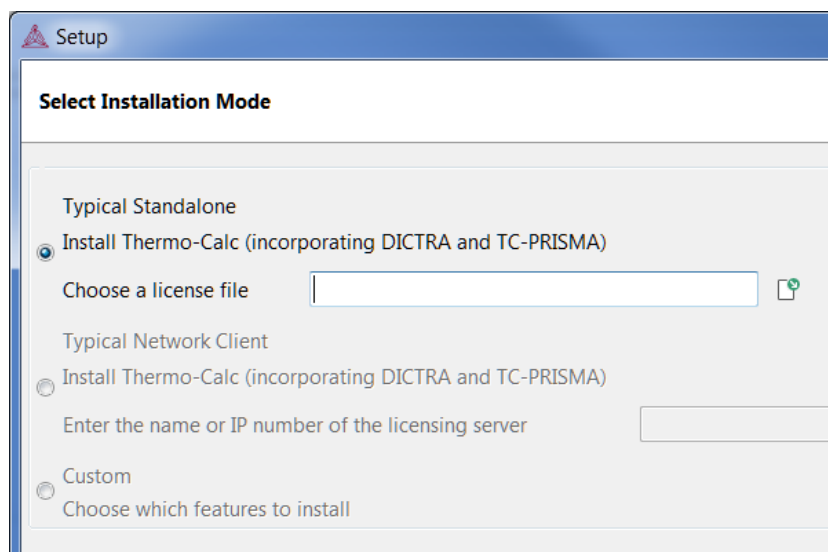
1. Download the software:
  - *Web downloads*: For web links sent in an email from Thermo-Calc Software, go to the URL and log in with the information provided to download the software.
  - *DVD installations*: Insert the DVD and follow the instructions.
2. Open the Mac folder and right-click the file **Thermo-Calc-2016a-osx.app**. Choose **Download Linked File** and save the installation file to your **Downloads** directory. Unzip the file.


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



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

### Step 3: Select the installation mode



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



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

3. The installation starts and is done when the **Completing the Thermo-Calc Setup Wizard** window opens.
4. Click **Finish** and start using Thermo-Calc.

# **Installation Guide for all Platforms**

**Windows®, Mac OS® or Linux Operating Systems**

**Version 2016a**



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# Installing Thermo-Calc

In this section:

---

<i>System Requirements</i> .....	3
<i>Key to Using this Guide</i> .....	3

## System Requirements

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

Additional components include:

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

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

- TQ-Interface (Windows and Linux)
- TC-API (Windows and Linux)
- TC-Toolbox for MATLAB<sup>®</sup> (Windows only)



System requirements and program availability are available on the web:

<http://www.thermocalc.com/products-services/software/system-requirements/>

## Platforms Tested

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

Windows	Mac	Linux <sup>1, 2</sup>
Windows 10 64-bit Windows 8 64-bit Windows 7 SP1 32-bit Windows 7 SP1 64-bit	Mac OS X El Capitan (10.11.5)	<ul style="list-style-type: none"> <li>• Ubuntu 16.04 (Xenial)</li> <li>• CentOS 7.0</li> <li>• OpenSUSE 13.2</li> </ul>
<sup>1</sup> Thermo-Calc Software cannot guarantee full functionality if the software is installed on other Linux distributions.		
<sup>2</sup> If you are installing on CentOS 7, it is recommended you install gtk2 before you run the installation script.		





## Key to Using this Guide

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

This guide includes information about:

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

## Icons

Name	Description
Information	 Provides important information and indicates that more detail is located in the linked or named topic.
Note	 The information can be of use to you. It is recommended that you read the text or follow the link to more information.
Operating system	The information is specific to a Windows, Mac OS or Linux operating system. In some cases, when there are minor differences, only the platform name is used, e.g. <i>Windows</i> only.
 License file	The license file, which contains the license keys and is installed on either a standalone computer or a network server.
 Thermo-Calc	The Thermo-Calc software and its components (including databases) to be installed.

## Typographical Conventions

Convention	Definition
Forward arrow →	The forward arrow symbol > instructs you to select a series of menu items in a specific order. For example, <b>Tools→Options</b> is equivalent to: From the <b>Tools</b> menu, select <b>Options</b> .
<b>Boldface font</b>	A <b>boldface</b> font indicates that the given word(s) are shown that way in on a toolbar button or as a menu selection. For example, if you are told to select a menu item in a particular order, such as <b>Tools→Options</b> , or to click <b>Save</b> .
<i>Italic font</i>	An <i>italic</i> font indicates the introduction of important terminology. Expect to find an explanation in the same paragraph or elsewhere in the guide.

Convention	Definition
<code>code</code> and <b>code bold</b>	A <code>code</code> font indicates you are to make a keyboard entry. It also shows a programming code or code examples. The <b>code bold</b> font highlights the entry.

## Terminology

Term	Definition
client computer	A computer without a license file of its own but connected through the network to a computer with the license information. The client computer receives a license token from the computer where the license management software is installed.
consolidated network	A type of network installation where the Thermo-Calc software and a Thermo-Calc licensing software are installed on a single server computer. This allows all computers in the network to access both the software and a license on the server via a client installation.
distributed network	A type of network installation where the Thermo-Calc software is installed on one server computer in a network and the Thermo-Calc licensing software is installed on a different computer. After a thin client installation, all computers in the network can access both the software and the network license key via the server.
host ID	The MAC/Ethernet Address on the computer that a license is locked to.
license file	The file (called <i>lservrc</i> ) that contains all the purchased license keys. It is issued by Thermo-Calc Software, usually by email.
license key	The information contained in the license file that represents the products purchased and which is then authorised for installation.
License Manager (Windows)	The Windows program used for license management: it distributes license tokens as specified in the network license file issued by Thermo-Calc Software.
License Server (Linux)	The Linux program used for license management: it distributes license tokens as specified in the network license file issued by Thermo-Calc Software.
license server	The use of the term <i>license server</i> (lower case letters) is reserved for use for scripts and option files (for example, in an <a href="#">Unattended Network Client Installations on page 35</a> ). For the purposes of the step-by-step instructions it is not used to refer to the type of network installation that runs the license management program. Also see <i>License Manager</i> (Windows) and <i>License Server</i> (Linux).
licensing software	The Thermo-Calc license management software. When working in Windows it is called <i>License Manager</i> (full name is Sentinel RMS License Manager by SafeNet) and on Linux it is called <i>License Server</i> (full name is Sentinel License Server by Safenet).



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

---

# License and Installation Types

In this section:

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<i>License and Installation Types</i> .....	8
<i>About License Keys and Files</i> .....	8
<i>Standalone Installations (SUNLL)</i> .....	8
<i>Multi-User Network Installations (NWL)</i> .....	9

## License and Installation Types

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



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

License type	Installation Type	Windows	Mac OS	Linux
SUNLL	Standalone	Yes	Yes	Yes
NWL	Consolidated network	Yes	No	Yes
	Distributed network	Yes	No	Yes
	License installations on a server network	Yes	Yes <sup>1</sup>	Yes

<sup>1</sup> For Mac OS, the licensing software is installed on a Windows or Linux computer server.



[www.thermocalc.com/purchase/licensing-options/](http://www.thermocalc.com/purchase/licensing-options/)

## About License Keys and Files



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



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

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



*Request a License File from Thermo-Calc Software on page 38*

## Standalone Installations (SUNLL)

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



To get started, go to [First Steps of Installation](#) on page 13 and then [Standalone Installations](#) on page 20.

## Multi-User Network Installations (NWL)

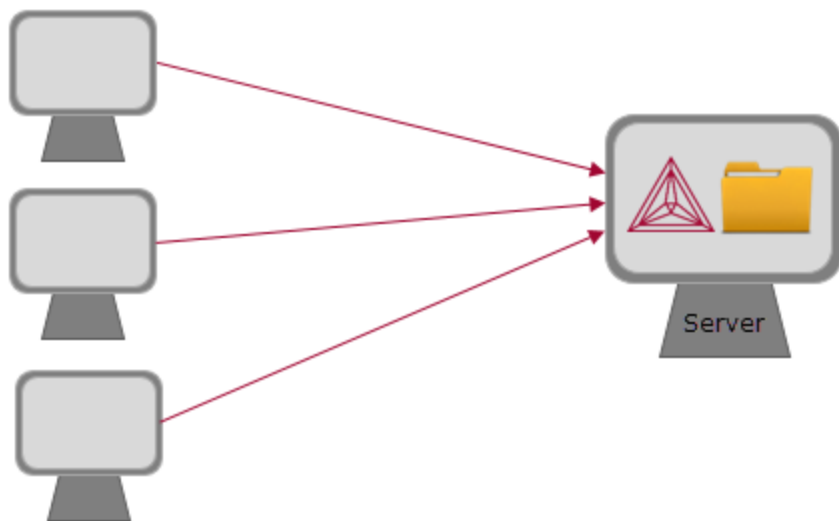
There are different types of multi-user network installations: consolidated, distributed and where the licensing software is installed on a computer network. There is also a subtype of installation called thin client, which is a step done with the consolidated and distributed network installations.





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

### Consolidated Network Installations

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

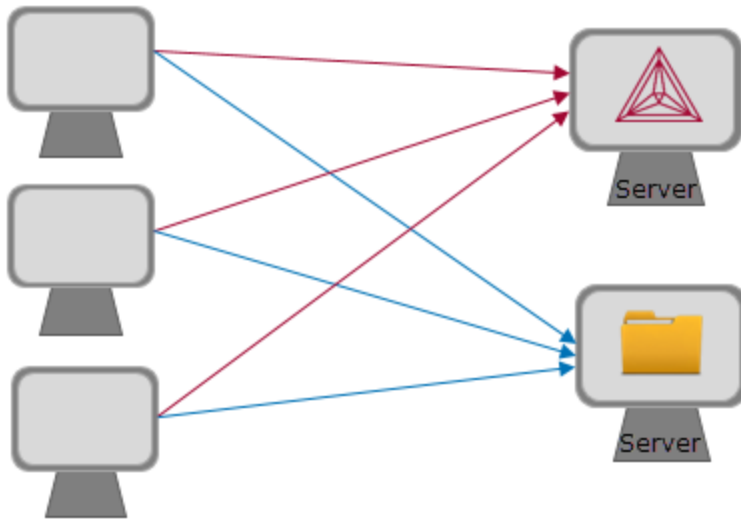




The Thermo-Calc software  and the license management program are installed on the same server where the license file  is also copied. A thin client installation allows all computers (the clients) in the server network to access both the software and the licensing on the same computer server.

To get started, go to [First Steps of Installation on page 13](#) and then [Network Client Installations on page 26](#).

## Distributed Network Installations

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

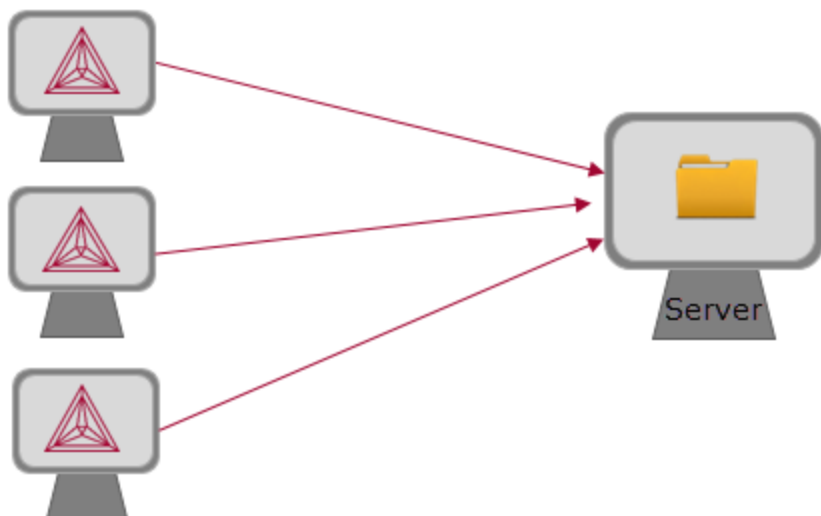




The Thermo-Calc software  is installed on one computer server in a network and the licensing software is installed on a different computer server where the license file  is also copied. A thin client installation allows all computers (the clients) in the server network to access both the software and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

To get started, go to [First Steps of Installation on page 13](#) and then [Network Client Installations on page 26](#).

## License Installations on a Server Network

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



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

To get started, go to [First Steps of Installation on page 13](#) and then [Network Client Installations on page 26](#).

---

# Preparing for Installation

In this section:

---

<i>First Steps of Installation</i> .....	<a href="#">13</a>
<i>Default Directory Locations</i> .....	<a href="#">13</a>
<i>Subnet Information for Network Licenses</i> .....	<a href="#">16</a>
<i>Mac OS Installation Notes</i> .....	<a href="#">17</a>
<i>Linux Installation Notes</i> .....	<a href="#">18</a>

## First Steps of Installation

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

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

```
yum install gtk2
```



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

## Default Directory Locations

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



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

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

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



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

## TC-Toolbox for MATLAB

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

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

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

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

## Database Checker Program

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

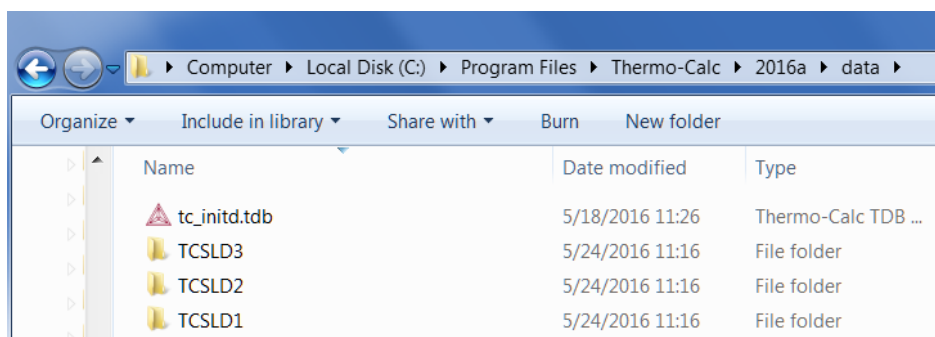


Thermo-Calc accepts deviations from these syntax rules. This means that a database can work even if the Database Checker reports errors and warnings. For example, an error is reported if an abbreviated phase name is found, but phase name abbreviations are accepted by Thermo-Calc and its add-on modules.

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

## Databases

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



## Subnet Information for Network Licenses

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

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

- *Windows*: `ipconfig /all`
- *Mac / Linux*: `ifconfig`

## Mac OS Installation Notes

### Restarting After an Installation

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

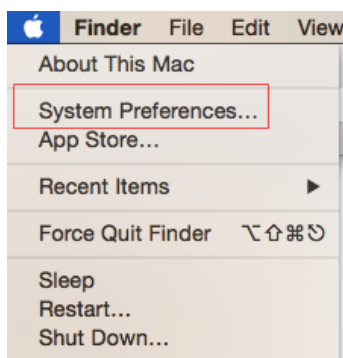
### Installing XQuartz

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

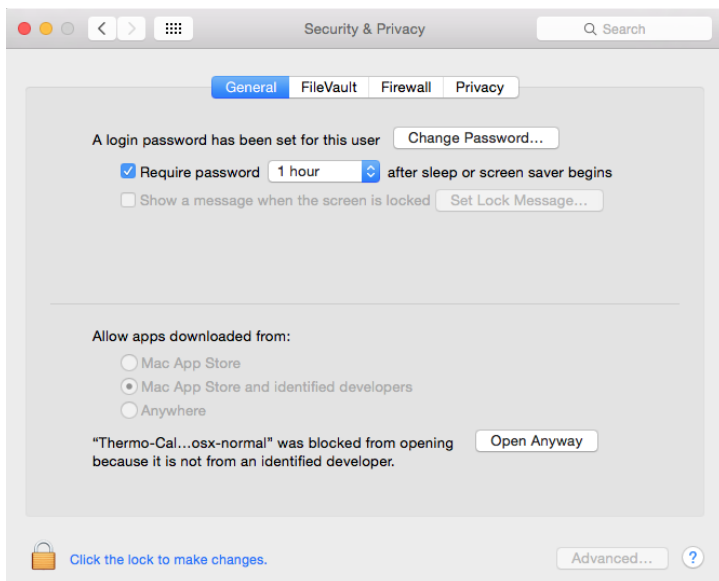
1. In a web browser go to <https://www.macupdate.com> or to download it directly from XQuartz, <http://xquartz.macosforge.org/landing/>.
2. In the **Search Mac Apps** field, enter *XQuartz*.
3. Click the **XQuartz** search result. For example, based on the recent version, the name is XQuartz-2.7.7.dmg.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

### Enabling the Correct Security Settings

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



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



4. If you have already tried to launch the Thermo-Calc installer, you can click **Open Anyway** to proceed. Otherwise, under **Allow apps downloaded from:** click **Anywhere** and then **Allow from Anywhere**.
5. Continue with the applicable installation type (standalone or network).



Remember to reset your security after installing Thermo-Calc.


## Linux Installation Notes

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

### Installing Libgfortran

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

#### How to install the runtime library

Linux distribution	Notes
openSUSE 13.2	 On a standard installation, you do not need to install this runtime library. You may need GCC if it is not already installed on your computer.
Ubuntu 16.04 (Xenial)	Open a terminal and enter the following: <pre>&gt; sudo apt-get -y update</pre> <pre>&gt; sudo apt-get -y install gfortran</pre>
CentOS 7.0	Open a terminal and enter the following: <pre>&gt; sudo yum -y update</pre> <pre>&gt; sudo yum -y install libgfortran</pre>

## openSUSE Administration (sudo) Users

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

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

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

## Opening Thermo-Calc in Linux

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

---

# Standalone Installations

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

In this section:

---

<i>Typical Standalone Installations</i> .....	<a href="#">21</a>
<i>Add New Components to an Existing Installation</i> .....	<a href="#">23</a>
<i>Custom Standalone Installation</i> .....	<a href="#">23</a>

---

## Typical Standalone Installations

The following describes a typical standalone installation. These steps assume you have completed the section *First Steps of Installation* on page 13.

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



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



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

Follow the instructions for your operating system in the section *Request a License File from Thermo-Calc Software* on page 38.

### Step 2: Download your Thermo-Calc installation software

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

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

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

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



If you are an openSUSE root user, see *Linux Installation Notes* on page 18 for some information about your installation.



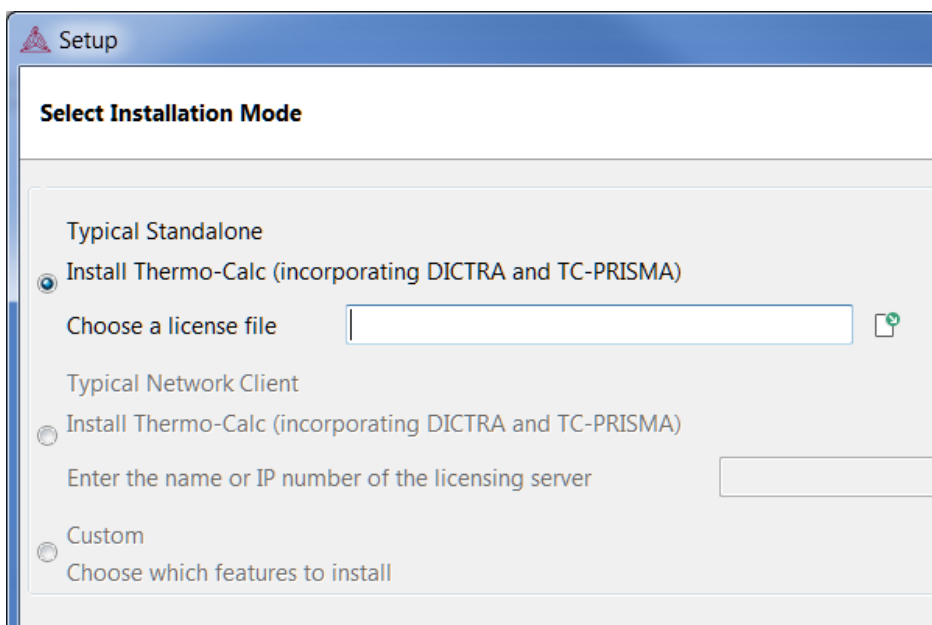
2. On the **Setup-Thermo-Calc** window click **Next**.
3. On the **License Agreement window** click to accept the license agreement.
4. Click **Next**.




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

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

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



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



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

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

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



If you did not get your license file see [Request a License File from Thermo-Calc Software on page 38](#).

## Add New Components to an Existing Installation

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

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



Use the **Uninstall** program to *remove* components. See [Uninstalling Thermo-Calc on page 57](#).

## Custom Standalone Installation

This topic describes how to do a custom installation on a standalone computer for either a Windows or Linux operating system. These steps assume you have completed the section [First Steps of Installation on page 13](#).

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

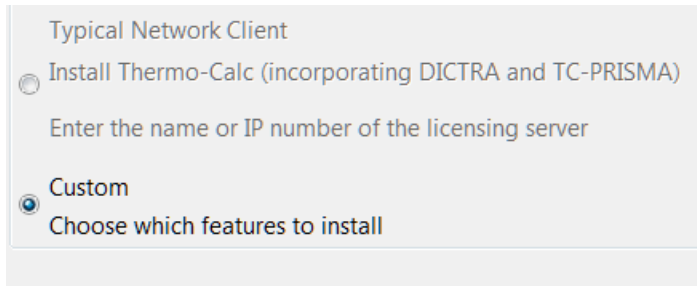
Follow the instructions for [Typical Standalone Installations on page 21](#) to get your license file and to download and run the software.

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

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



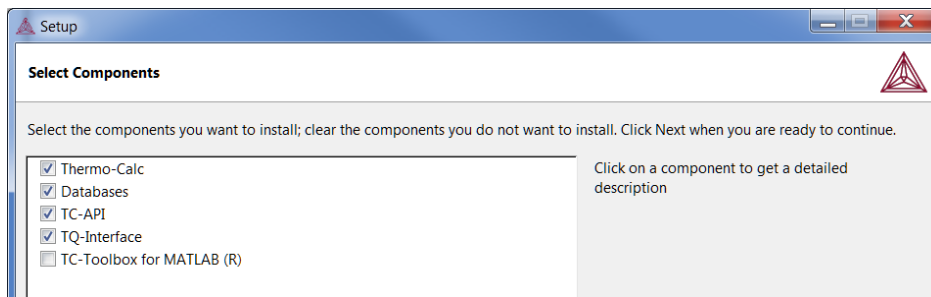
The option appears greyed out, but it is available to select.




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

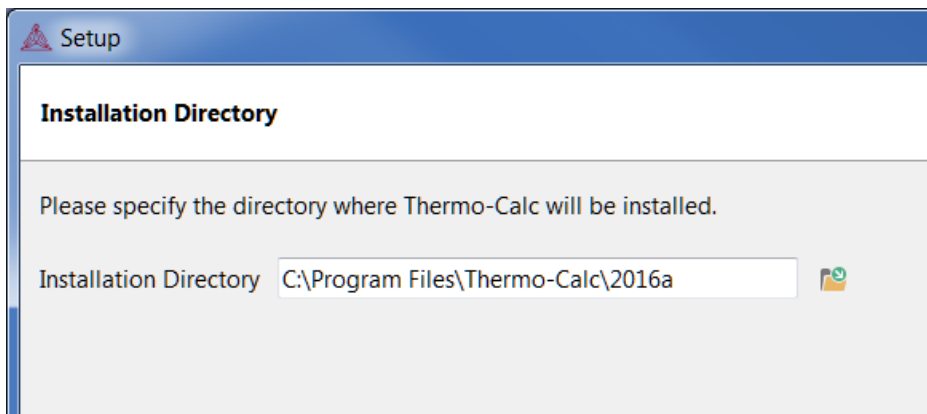


Additional licenses are required to run TC-API, TQ-Interface, TC-Toolbox for MATLAB (Windows only) and some of the databases. Some elements are included with Precipitation Module (TC-PRISMA) but a separate license is required for full functionality.




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

1. In the **Installation Directory** window, either accept the default path or enter a path to where you want to install the software (see [Default Directory Locations](#) on page 13). Click the file button  to navigate to another directory. Click **Next**.

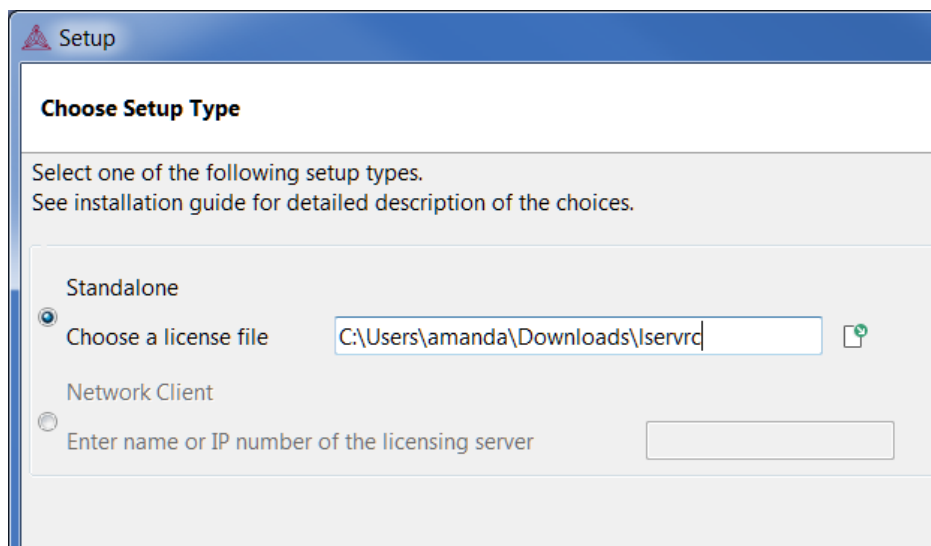


For the Windows TC-Toolbox for MATLAB® component, and if you get a **MATLAB not found** message, enter the MATLAB installation directory and click **Next**.

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



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



4. Set up the Desktop shortcuts.

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

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

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

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



If you did not get your license file see [Request a License File from Thermo-Calc Software on page 38](#).

---

## Network Client Installations

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

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

In this section:

---

<i>Typical Network Client Installations</i> .....	<a href="#">27</a>
<i>Set Up the License Manager on Windows</i> .....	<a href="#">28</a>
<i>Set Up the License Server on Linux</i> .....	<a href="#">29</a>
<i>Thin Client Installations</i> .....	<a href="#">31</a>
<i>Custom Network Client Installations</i> .....	<a href="#">33</a>
<i>Unattended Network Client Installations</i> .....	<a href="#">35</a>

## Typical Network Client Installations

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

### Step 1: Install the licensing software

Follow the instructions for your operating system:

- *Set Up the License Manager on Windows* on the next page, or
- *Set Up the License Server on Linux* on page 29

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

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

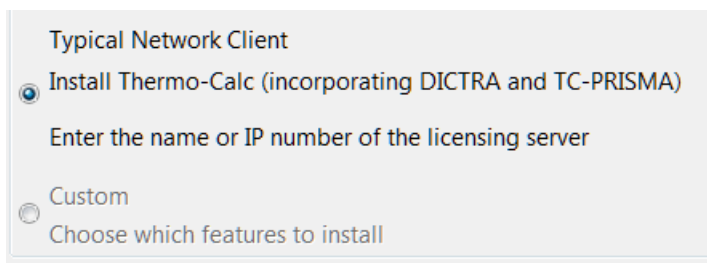
### Step 3: Choose the installation type and enter the computer server details

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



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

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



### Step 4: Install the software and components

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



If you did not get your license file see [Request a License File from Thermo-Calc Software](#) on page 38.

## Set Up the License Manager on Windows



**License Manager vs License Server:** Both terms refer to the licensing software program installed on a network computer. License Manager is for Windows and License Server is for Linux.

### Installation Requirements

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

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

### Installing the License Manager

#### Step 1: Install the Sentinel RMS License Manager software

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

#### Step 2: Choose the installation directory

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

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

### Step 3: Choose the setup type and install the software

1. In the **Setup Type** window, select **Complete**. Click **Next**.
2. In some cases, select **Unblock the system firewall for the Sentinel RMS License Manager**. This changes the settings to allow the License Manager to communicate with the computers running the client applications. Click **Next**.
3. Click **Install**.
4. Click **Finish** to exit the InstallShield Wizard.

### Step 4: Copy the license files to the destination directory

1. Copy the network license file to the destination directory. By default, it is installed in this directory:

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

You can also set the environmental variable **LSERVOPTS** to the complete path and name of the LSERVRC license file:

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

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

## Set Up the License Server on Linux



**License Manager vs License Server:** Both terms refer to the licensing software program installed on a network computer. License Manager is for Windows and License Server is for Linux.

## Installation Requirements

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



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

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

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

### openSUSE Administration (sudo) Users

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

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

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

### Installing the License Server

#### Step 1: Stop any older versions of the License Server



Skip this step if this is a new installation.

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

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

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

#### Step 2: Write a script to start the License Server

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

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

```
# set the directory where the executables are located
LICENSE_SERVER_DIR=/usr/local/Thermo-Calc/2016a/Licensing-files
```

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

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

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

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

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

### Step 4: Start the License Server

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

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

## Thin Client Installations

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

## Installation Requirements

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

### Installing a Thin Client on Windows

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

### Installing a Thin Client on Linux

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

```
[public]
path=/home/<user>/Thermo_Calc/2016a
public=yes
writable=yes
comment=smb share
guest OK=yes
force user=<user>
```

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

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

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

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

```
> ./client-install-linux-x64.run
```
5. Click **Forward** and click to select the license agreement. Click **Forward**.
6. Enter the name or IP number of the License Server. Click **Forward**.
7. If you are installing as a non-root user, by default, the **Create Shortcuts on Desktop** check box is selected. Click **Forward**.
8. In the **Ready to Install** window click Forward.
9. Click **Finish**. Log out and log back in to start using Thermo-Calc.

## Custom Network Client Installations

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

### Step 1: Install the licensing software

Follow the instructions for your operating system:

- [Set Up the License Manager on Windows on page 28](#), or
- [Set Up the License Server on Linux on page 29](#)

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

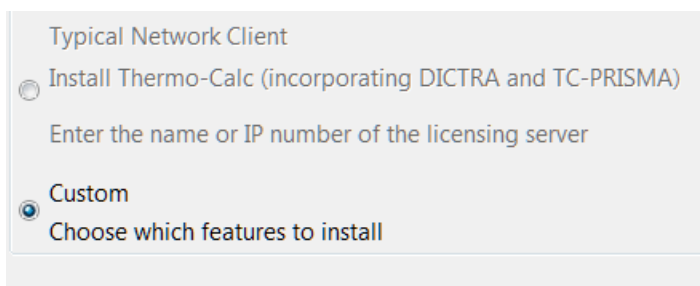
Follow the instructions for [Typical Standalone Installations on page 21](#) to download and run the software. It is up to you whether you get the computer information for the license files before or after installing the software.

### Step 3: Choose the installation type and what to install

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



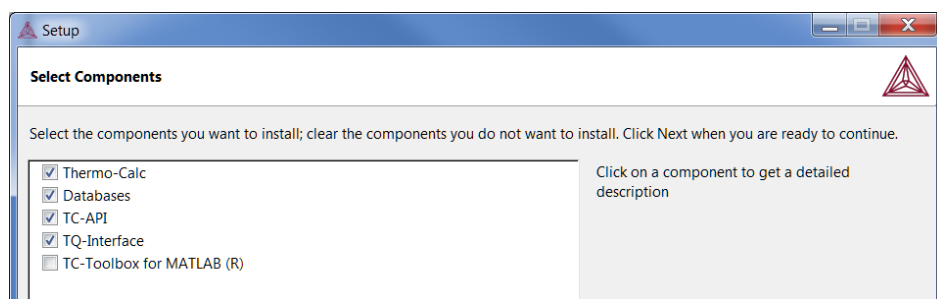
The option appears greyed out, but it is available to select.



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

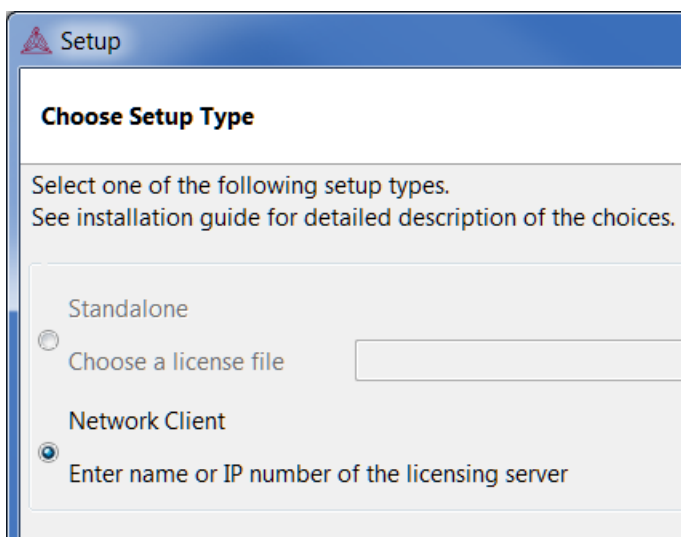
#### Step 4: Set the installation directory path to the license file

1. In the **Installation Directory** window, enter the path to an installation directory (see *Default Directory Locations* on page 13). Click **Next**.



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

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



## Step 5: Specify the configuration and create shortcuts

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

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

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

1. In the **Ready to Install** window click **Next**.
2. When the **Completing the Thermo-Calc Setup Wizard** window opens, click **Finish**.
3. Log out and log back in and start using Thermo-Calc. If you have not got the license file, go to [Request a License File from Thermo-Calc Software on page 38](#).

## Unattended Network Client Installations



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

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



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

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

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

```
installation_mode=custom
setup_type=client
enable-components=thermo,tcprisma,databases,tq,tcapi,toolbox
config=all
icons=1
license_server=<name/IP number>
```

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

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

```
installation_mode=typical_client
```

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

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



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

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

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

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

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

---

## Request License Files

In this section:

---

<i>Request a License File from Thermo-Calc Software .....</i>	<i>38</i>
<i>Getting License Information Using Thermo-Calc .....</i>	<i>38</i>
<i>Requesting the License File for Windows .....</i>	<i>39</i>
<i>Requesting the License File for Mac OS .....</i>	<i>41</i>
<i>Requesting the License File for Linux .....</i>	<i>42</i>



## Request a License File from Thermo-Calc Software

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

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

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



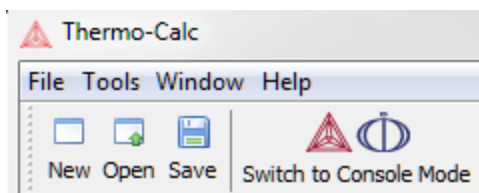
<http://www.thermocalc.com/support/request-support/>

## Getting License Information Using Thermo-Calc

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

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

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



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



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

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

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

## Requesting the License File for Windows

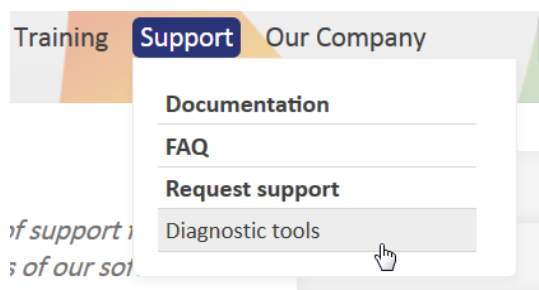


**Demo (trial) installations:** Skip this section. A license file is automatically installed with the software. You do not need to request it.

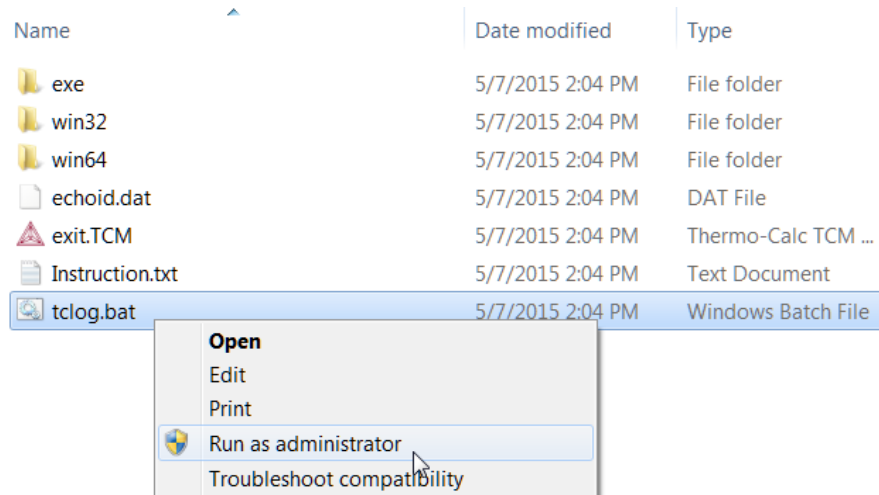


**Upgrades to a new version of Thermo-Calc:** Skip this section if you are upgrading to a new version of Thermo-Calc and (and you have a maintenance plan). Your license is sent to you in an email from Thermo-Calc Software AB. Save it to your computer to use during software installation.

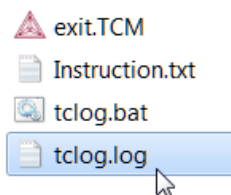
1. Go to Thermo-Calc's [website](#) (or click the link sent by email).



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



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



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

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

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



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

## Requesting the License File for Mac OS



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

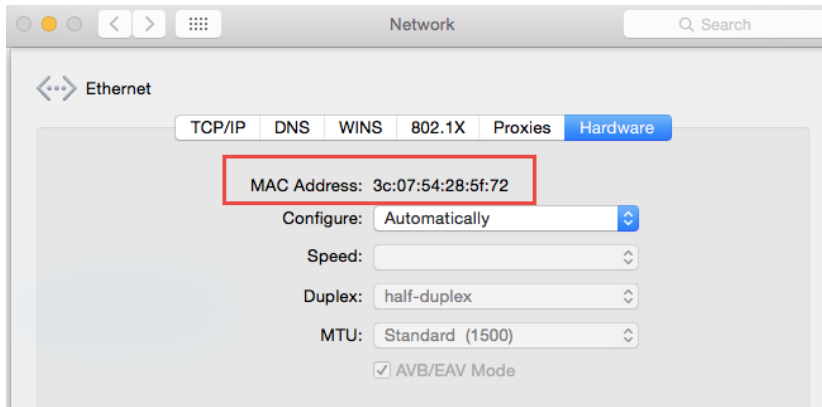


**Upgrades to a new version of Thermo-Calc:** Skip this section if you are upgrading to a new version of Thermo-Calc and (and you have a maintenance plan). Your license is sent to you in an email from Thermo-Calc Software AB. Save it to your computer to use during software installation.

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



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



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

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

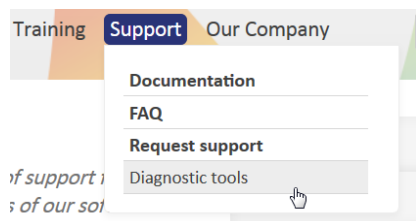
Designated Site 12345  
XYZ Company  
Dpt. of Material Science  
900 Main Street  
Stockholm 11190  
SWEDEN



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

## Requesting the License File for Linux

1. Go to Thermo-Calc's [website](#).
2. From the **Support** menu select **Diagnostic tools**.



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

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

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

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

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

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

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

To:

Cc:

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

Add attachments

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

---

## Troubleshooting

In this section:

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<i>License Errors</i> .....	<i>45</i>
<i>Determining the Current License File Directory Path</i> .....	<i>46</i>
<i>Specifying a New Server Name or IP Number</i> .....	<i>49</i>
<i>MATLAB® Installation Directory</i> .....	<i>50</i>
<i>Firewalls</i> .....	<i>51</i>
<i>Client/Server Mismatch</i> .....	<i>51</i>
<i>Mac OS Installations: Running the License Initialization Script</i> .....	<i>53</i>
<i>Linux Installations: Running the License Initialization Script</i> .....	<i>54</i>

## License Errors

Issue	Platform	Installation type	Action or link to more information
How do I add or update a standalone (SUNLL) license on a Windows computer where Thermo-Calc is already installed?	Windows	Standalone	<a href="#">Determining the Current License File Directory Path</a> on the next page
How do I add or update a standalone (SUNLL) license on a Linux computer where Thermo-Calc is already installed?	Linux	Standalone	<a href="#">Determining the Current License File Directory Path</a> on the next page
How do I add or update a network license on Windows?	Windows	Network	<a href="#">Determining the Current License File Directory Path</a> on the next page
How do I add or update a network license on Linux?	Linux	Network	<a href="#">Determining the Current License File Directory Path</a> on the next page
No license file found. Copy a valid license file to the installation directory after completing the installation.	All	All	You get this message if the wrong path or no license file is found at a path entered during the installation process. See <a href="#">Default Directory Locations</a> on page 13 and <a href="#">Determining the Current License File Directory Path</a> on the next page
MATLAB not found (for the TC-Toolbox for MATLAB component)	Windows	All	<a href="#">MATLAB® Installation Directory</a> on page 50
Warning Environment variable “LSHOST” is not set. Software will not function properly.	All	Network	<a href="#">Specifying a New Server Name or IP Number</a> on page 49
Problem running post-install step. Installation may not complete correctly.	Linux and Mac	Standalone	<a href="#">Mac OS Installations: Running the License Initialization Script</a> on page 53 or <a href="#">Linux Installations: Running the License Initialization Script</a> on page 54



Issue	Platform	Installation type	Action or link to more information
Unable to run post-installation script, run the license initialization script as root after the installation.			
Firewall warnings related to license management software (License Manager and License Server)	Windows and Linux	Network	<a href="#">Firewalls on page 51</a>
Client / Server naming mismatches	Windows and Linux	Network	<a href="#">Client/Server Mismatch on page 51</a>
InstallScript engine missing	Windows	Network	You are not notified if the InstallScript scripting engine is not installed. Install the ISScript.msi file and then run the downloaded file from Thermo-Calc again as described in <a href="#">Set Up the License Manager on Windows on page 28</a>

## Determining the Current License File Directory Path

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

### *From Thermo-Calc*

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

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

### Windows Standalone Installations

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

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

```
>set LSERVRC
```

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

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

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

## Linux Standalone Installations

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

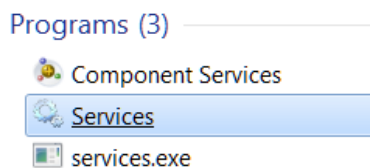
Find out where to place the new license file by opening a Terminal window and type in the command line:

```
echo $LSERVRC
```

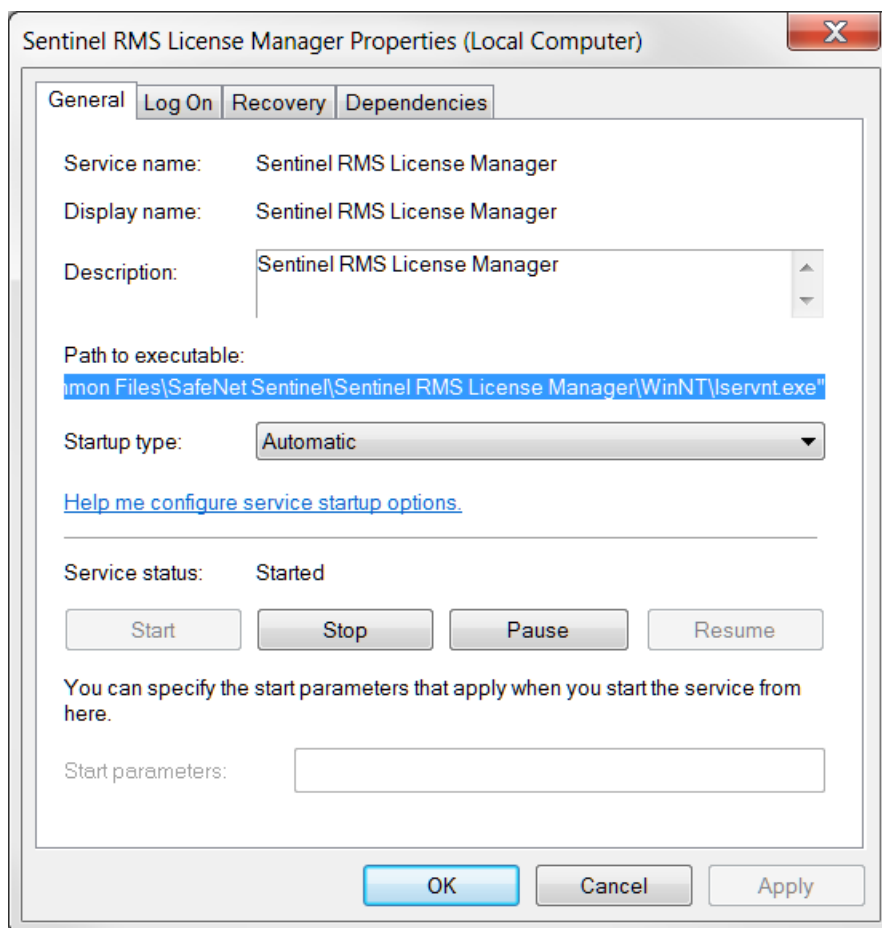
## Windows Network Installations

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

1. You need administrator rights to do the following.
  - On *Windows 7*, click the Start button and in the search field type **Services**. Double-click the **Services** result.



- On *Windows 8*, move the mouse over the right edge of the screen to access Search, click Settings and then enter and select **View Local Services**.
2. In the list of installed services, right-click **Sentinel RMS License Manager** and select **Properties** from the pop-up menu.
  3. On the **General** tab under **Path to executable**, click the line containing the path to see where the file **lservnt.exe** is located. The license file (**lservrc**) is in the same directory.



The default path for the license file is

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

4. Move your copy of the license file (lservrc) to this directory.
5. Restart the Sentinel RMS License Manager by:
  - Restarting the computer, or
  - Right-clicking **Sentinel RMS License Manager** and selecting **Restart** from the list of installed services.

## Linux Network Installations

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

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

## Specifying a New Server Name or IP Number

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

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

## Windows

### Changing the server name or address (Windows)

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

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

1. Close all running Thermo-Calc programs.
2. Open a command line window.
  - In *Windows 8*, use Search (mouse-over the right edge of your screen) to find **cmd** and then double-click the Command line icon.
  - In *Windows 7*, from the Start menu click **Run** and type **cmd** in the field.
3. Specify the name or IP number of the licensing software server. Type:

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

To display the current name or IP number, type:

```
set LSHOST
```

## Mac

### Mac installations

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

In this file, you can manually set the `TC60_HOME` variable, which specifies the home directory of the Thermo-Calc program. See the `plist.info` file for an example.

## Linux

### Linux installations

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

### MATLAB® Installation Directory

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

### Determining the licensing software version

Sometimes you may need to know the version of License Manager (Windows) or License Server (Linux)

software being used. This can be useful while troubleshooting network installations.

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

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

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

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

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

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

## Firewalls

### Windows

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

### Linux

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

## Client/Server Mismatch

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

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

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

### How to Check

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

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

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

- Host name
- Dns Suffix
- Current IPv4 Address

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

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

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

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

#### *Step 2: Try these options to correct the issue*

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

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

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

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

## **Mac OS Installations: Running the License Initialization Script**

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



## How to Run the Script

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



Also see [Default Directory Locations](#) on page 13.

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

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

For demo installations, the path should be /Applications/Thermo-Calc-2016a-Demo.app/Contents/Resources/ license-initialization-MacOS-x86\_64.sh.

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

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



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

## Linux Installations: Running the License Initialization Script

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

### openSUSE Administration (sudo) Users

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

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

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

## How to Run the Script



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



Also see [Default Directory Locations](#) on page 13.

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

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

2. Enter this command:

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

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

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

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

---

# Uninstalling Thermo-Calc

In this section:

---

<i>Uninstalling Thermo-Calc</i> .....	<i>57</i>
<i>Uninstalling Standalone Versions of TC-PRISMA</i> .....	<i>59</i>

## Uninstalling Thermo-Calc

## Windows

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

## Mac

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

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

## Linux

1. To start the uninstallation procedure, in the Thermo-Calc installation directory use the command

```
./uninstall-Thermo-Calc-2016a
```

For *Thin Client* installations, use the command `/uninstall-Thermo-Calc-Client-2016a`

2. To remove the whole application, including all its components, select **Entire application** and click **Forward**, or to remove specific components, select **Individual components** and click **Forward**.



If you intend to reinstall Thermo-Calc 2016a it is important to remove the environmental variable TC60\_HOME by logging out and back into the Linux user account.

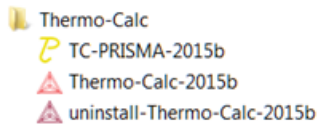
## Uninstalling Standalone Versions of TC-PRISMA



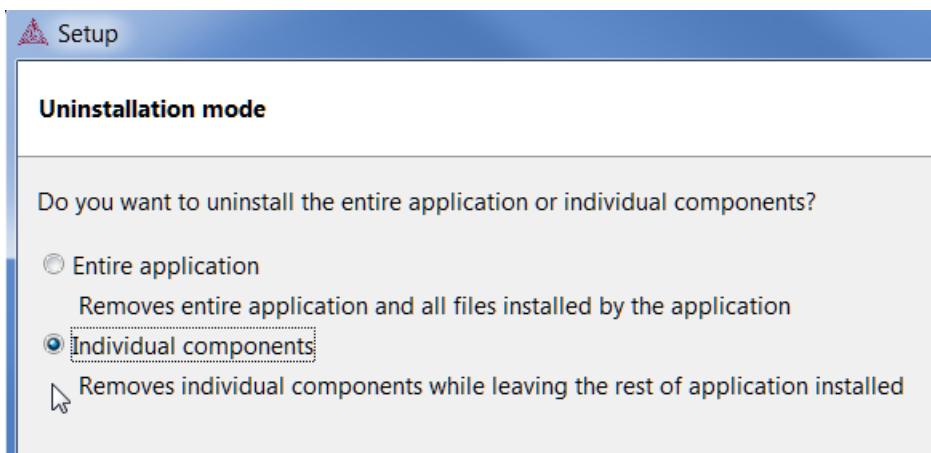
As of Thermo-Calc version 2016a, TC-PRISMA is no longer a standalone program. It is integrated into the Thermo-Calc Graphical Mode and considered an add-on module called the Precipitation Module. It is also available for all platforms (Windows, Mac and Linux). If you have older versions of the TC-PRISMA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

1. Go to the Thermo-Calc uninstaller. For example, in Windows 7, go to **Start>All Programs>Thermo-Calc**.

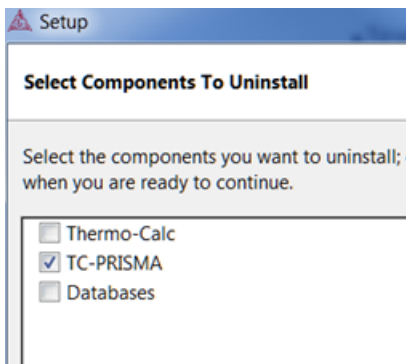
2. Click **uninstall-Thermo-Calc-2015b** (or the version of TC-PRISMA you have).



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



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



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

# Thermo-Calc User Guide

Version 2016a





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# Introduction to Thermo-Calc

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

In this section:

---

<i>The Thermo-Calc Software</i> .....	3
<i>Typographical Conventions</i> .....	3
<i>Graphical Mode vs Console Mode</i> .....	4
<i>Help Resources</i> .....	5
<i>Examples, Documentation and Materials</i> .....	7
<i>The Thermo-Calc Modules and Activities</i> .....	20
<i>Displaying Thermo-Calc License Information</i> .....	23
<i>Using This Guide</i> .....	24

## The Thermo-Calc Software

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

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

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

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

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

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







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

## Typographical Conventions

The following typographical conventions are used throughout the documentation:

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

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

## Graphical Mode vs Console Mode

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

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

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

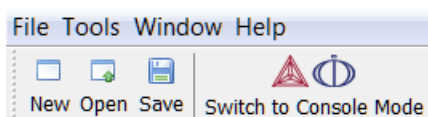
- In Console Mode you work with *modules*, which are managed using commands typed at a prompt. Some modules, called *response-driven modules*, prompt you with a series of questions that typically take you through the process of defining your system, setting calculation conditions, performing calculations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

## Switching Between Modes

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

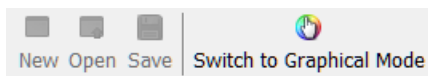
Along the top of the GUI is the toolbar where you switch between modes.

### The toolbar in Graphical Mode



### The toolbar in Console Mode

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



See [Main Menu and Toolbar on page 32](#) for information about the **Tools**, **Window** and **Help** menus, which are available in both modes.



The two modes can be run simultaneously, but there is no communication between them. What you do in Graphical Mode does not affect the state of the Console Mode session and vice versa. One exception is the plot settings. See [Global Settings: Graphical and Console Mode-Plotting on page 200](#).



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

## Help Resources

### Online and Context Help


#### Online Help

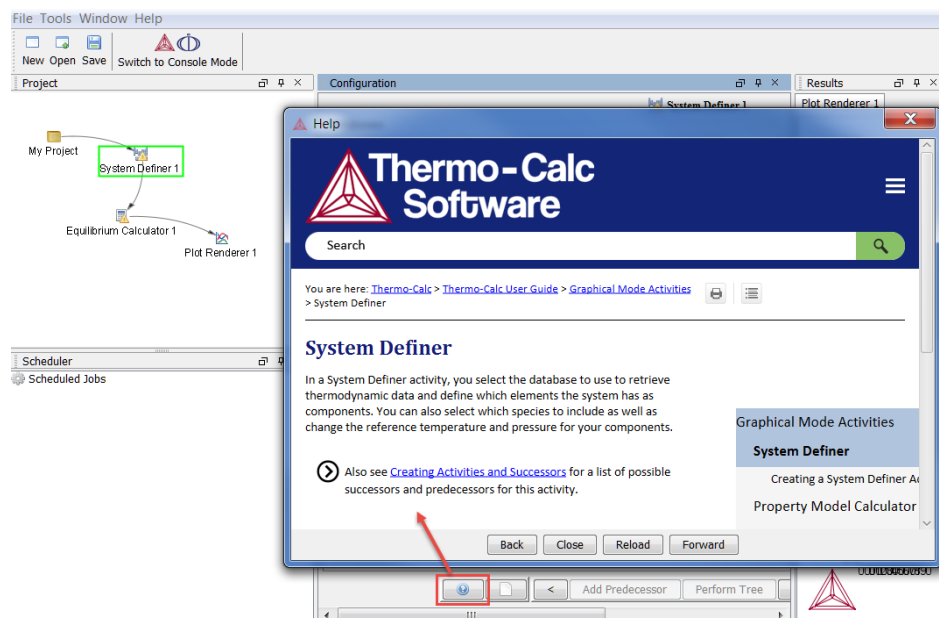
To access online help in a browser, open Thermo-Calc and select **Help → Online Help**. The content opens

in a browser but uses local content so you don't need an internet connection.





## Context Help

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

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



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

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

## Console Mode Help



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

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

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

## Examples, Documentation and Materials

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

## Installation Resources



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

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

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

## PDF Documentation

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

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

Guide.

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

## Database Information Sheets

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

## Graphical Mode Example Collection

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

### Opening a Project File

Navigate to the file location and double-click the \*.t<sub>cu</sub> file to open it. It launches a new session of the software. Or you can select **File →Open Project** from an open session of Thermo-Calc.



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

The project files have the extension \*.t<sub>cu</sub>.



- 
- ▲ Ex\_01\_Single-point\_equilibrium.tcu
  - ▲ Ex\_02\_Step\_in\_temperature\_in\_Fe-C.tcu
  - ▲ Ex\_03\_Fe-C\_phase\_diagram.tcu
  - ▲ Ex\_04\_Fe-Cr-C\_ternary\_phase\_diagram.tcu
  - ▲ Ex\_05\_Fe-C\_stable\_and\_metastable\_phase\_diagram.tcu
  - ▲ Ex\_06\_Serial\_equilibrium\_calculators.tcu
  - ▲ Ex\_07\_User\_defined\_functions.tcu
  - ▲ Ex\_08\_Scheil\_and\_equilibrium\_solidification.tcu
  - ▲ Ex\_09\_Heat\_map\_of\_carbide\_driving\_force.tcu
  - ▲ Ex\_10\_Phase\_Transition.tcu
  - ▲ Ex\_11\_Coarsening\_and\_Interfacial\_energy.tcu
  - ▲ Ex\_12\_Driving\_force\_and\_Interfacial\_energy.tcu
  - ▲ Ex\_13\_Precipitation\_Al-Sc\_AL3SC.tcu
  - ▲ Ex\_14\_Precipitation\_Fe-C-Cr\_Cementite-M7C3-M23C6.tcu
  - ▲ Ex\_15\_Precipitation\_Fe-C-Cr\_TTT\_Cementite-M7C3-M23C6.tcu
  - ▲ Ex\_16\_Precipitation\_Fe-C\_Cementite.tcu
  - ▲ Ex\_17\_Precipitation\_Ni-Al-Cr\_Isothermal\_Gamma-Gamma\_prime.tcu
  - ▲ Ex\_18\_Precipitation\_Ni-Al-Cr\_Non-isothermal\_Gamma-Gamma\_prime.tcu

## Examples of Thermo-Calc Activities

### Example 1: Calculating a Single-Point Equilibrium

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

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

The displayed results of the calculation show that the BCC\_A2 (ferrite) and GRAPHITE phases are stable for this set of equilibrium conditions.

File Name	Activity Example
Ex_01_Single-point_equilibrium	Equilibrium Calculator

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

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

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

### Example 3: Fe-C Phase Diagrams

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

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

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

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

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

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

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

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

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

File Name	Activity Example
Ex_05_Fe-C_stable_and_metastable_phase_diagram	Equilibrium Calculator

#### Example 6: Serially Coupled Equilibrium Calculators

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

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

where only the FCC A1 and BCC A2 phases are stable. The results from this preliminary calculation are displayed in Table Renderer 1.

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

File Name	Activity Example
Ex_06_Serial_equilibrium_calculators	Equilibrium Calculator

### Example 7: User-Defined Functions

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

File Name	Activity Example
Ex_07_User_defined_functions	Equilibrium Calculator

### Example 8: Scheil and Equilibrium Solidification

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

File Name	Activity Example
Ex_08_Scheil_and_equilibrium_solidification	Scheil Calculator

### Example 9: Carbide Driving Force Heat Maps

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

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

File Name	Activity Example
Ex_09_Heat_map_of_carbide_driving_force	Plot Renderer

### Example 10: Phase Transition

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

File Name	Activity Example
Ex_10_Phase_Transition	Property Model Calculator

### Example 11: Coarsening and Interfacial Energy

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

File Name	Activity Example
Ex_11_Coarsening_and_Interfacial_energy	Property Model Calculator

### Example 12: Driving Force and Interfacial Energy

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

File Name	Activity Example
Ex_12_Driving_force_and_Interfacial_energy	Property Model Calculator

## Console Mode Example Collection

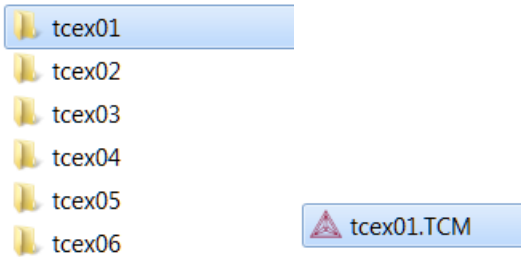
After you have accessed the [Examples, Documentation and Materials on page 7](#), go to the Console Mode Example folder to open one of the macro files in Thermo-Calc.

### Opening a Macro File

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

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

Name



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

### Console Mode Example Descriptions


#	Example Description
1	Calculation of the binary Fe-C phase diagram.
2	Plotting of thermodynamic functions in unary, binary and ternary systems and working with partial derivatives and partial quantities
3	Calculation of an isothermal section using the TERNARY module.
4	Calculation of the miscibility gap in Fe-Cr
5	Calculation of a vertical section from Al to 30% Mg <sub>2</sub> Si
6	<p>Calculation of an isopleth in low alloyed Fe-Mn-Si-Cr-Ni-C steel.</p> <p>This example calculates a multicomponent phase diagram using the define-material command in POLY and the TCFE steel database. The material contains 1.5 %Cr + 0.4 %Mn + 3.5 %Ni + 0.3 %Si and 1 %C (by weight). These conditions and the temperature are set by the command. Hidden commands set the pressure to 1 bar and so that iron is "the rest".</p> <p>After calculating the first equilibrium a phase diagram is calculated with one axis variable as temperature and the other as the carbon content.</p>
7	<p>Calculation of single equilibria in low alloyed Fe-Mn-Si-Cr-Ni-C steel. There are two general ways to perform a single equilibrium calculation:</p> <ul style="list-style-type: none"> <li>• Get data from a database, then in POLY use SET_CONDITION and COMPUTE_EQUILIBRIUM.</li> <li>• Go directly to POLY and use DEFINE_MATERIAL.</li> </ul> <p>The COMPUTE_TRANSITION command is also used to determine the temperature or</p>

#	Example Description
	composition where one phase forms or disappears.
8	Calculation of property diagrams for a high speed steel i.e. phase fraction plots, activity vs temperature, etc.
9	Calculation of dew point.
10	<p>The example calculates an equilibrium with suspended or dormant phases and shows how to avoid clogging of Cr<sub>2</sub>O<sub>3</sub> in a continuous casting process. The origin of this example is that a manufacturer wanted to increase the Cr content of a material from 18 to 25 weight percent but the continuous casting of this material was problematic because solid Cr<sub>2</sub>O<sub>3</sub> was formed. Using Thermo-Calc to calculate the equilibria in the steel/slag system, a simple correction was found: modify the Mn or Si content to decrease the oxygen potential.</p> <p>In Thermo-Calc, you can FIX a phase with zero amount to simulate how to avoid forming this phase. You then release one of the conditions, usually one of the compositions, and this composition is determined by the equilibrium calculation.</p>
11	<p>This example demonstrates the oxidation of Cu<sub>2</sub>S with H<sub>2</sub>O/O<sub>2</sub> gas mixture. Thermo-Calc is used to find the optimum O/H ratio (i.e. oxygen potential) as certain oxygen potential values can desulphurize Cu<sub>2</sub>S without forming copper oxides.</p> <p>In Thermo-Calc, the problem reduces to perform equilibria calculations in a Cu-S-H-O system. The amounts of the components should be kept to correct ratio corresponding to Cu<sub>2</sub>S and H<sub>2</sub>O using a command SET_INPUT_AMOUNTS in POLY_3. Initially, O/H = 0.5 is given. Optimum O/H ratio is calculated with the desired calculation conditions. For example, to simulate one phase disappearing, you can FIX the phase with zero amount.</p>
12	This example shows a number of independent cases using the TAB- module to tabulate thermodynamic data for reactions.
13	Binary calculation of Al-Ti phase diagram and G curve.
14	Calculation of heat and heat capacity variations during solidification of an Al-Mg-Si alloy.
15	<p>Solidification simulation of a Cr-Ni alloy using the SCHEIL module.</p> <p>There is no back diffusion in the solid.</p>
16	Calculation of the second order transition line in the Bcc field of the Al-Fe system.
17	<p>Calculation of pseudo- or quasi-binary phase diagram in the CaO-SiO<sub>2</sub> system.</p> <p>This database can be used both for pseudobinary systems like the one in this case, CaO-SiO<sub>2</sub>, or for full ternary systems like Ca-Fe-O.</p>
18	Calculation of the A3 temperature of a steel and the influence of each alloying element on this temperature.

#	Example Description
	A3 temperature is the temperature where ferrite starts to form from austenite. You can easily read A3 from an Fe-C phase diagram. But for complex multicomponent steels, no simple diagram can be used. This example shows how to calculate the A3 temperature of a steel. Using POLY, it is easy to find out the influence of each alloying element on A3 temperature. This information is useful if you want to modify the compositions of a steel but keep A3 unchanged.
19A	Mapping of univariant equilibria with the liquid in Al-Cu-Si. Part A. Step-by-step calculation using POLY.
19B	Mapping of univariant equilibria with the liquid in Al-Cu-Si. Part B. Using the TERNARY module, you can get the information on invariant reactions, such as temperature and compositions.
20	Calculation of adiabatic decompression in a geological system using the geochemical database.
21	Calculate a ternary isotherm in Fe-Cr-Ni with a user-defined database.
22	Calculation of a heat balance. In this case C <sub>3</sub> H <sub>8</sub> is burned in oxygen and the adiabatic flame temperature is calculated.
23	Calculation of a para-equilibrium and the T <sub>0</sub> temperature in a low alloyed steel.
24	<p>Simulation of the silicon arc furnace using the REACTOR module.</p> <p>This is a simple reactor model with output of gases at the top and output of condensed phases at the bottom. The gas phase from one segment flows to higher segments, 80 % reacts in the first above, 15% in the second above and 5 % in the third above.</p> <p>The condensed phases flow downwards and all of it goes to the next lowest segment. Heat can be added at any module. The only way to specify the initial state of the reactants added to the reactor is to specify their heat content.</p>
25	<p>Simulation of steel refining.</p> <p>Raw iron used to produce steel usually has high carbon and silicon content, which is why oxygen is blown into the furnace to burn off carbon. Lime (CaO) is added to form a slag with silica, and the slag can be removed. Alloying elements, such as Mn, Ni, Cr and V are added to produce the desired steel. Since the reaction between O and C increases the temperature, scrap iron is added in order to keep the temperature constant (it is assumed the furnace is isolated and no heat is lost to the environment). This is a typical steel refining process.</p> <p>This example simulates blowing oxygen into a liquid steel of one metric ton (1e6 grams) with 4 w/o C, 2 w/o Si and 1 w/o Mn. 100 moles of CaO (equivalent to 5.6 kg) is added. Keeping the enthalpy constant is the way to simulate the isolation of the furnace. The oxygen reacts with carbon and increases the temperature. After blowing a certain amount of oxygen, scrap iron is added to keep the temperature constant.</p>



#	Example Description
26	Example of plotting the partial pressures of a gas species along the solubility lines in the As-Ga phase diagram. The calculation makes it possible to monitor the input gases to a process of depositing solid AsGa.
27	CVD calculations
28	Example showing calculation of PRE (Pitting Resistance Equivalence) for a duplex stainless steel.
29	Calculation of speciation of a gas
30A	Scheil solidification simulation for Al-4Mg-2Si-2Cu alloy. Part A. Step-by-step calculation using POLY and the STEP_WITH_OPTION command, EVALUATE option.
30B	Scheil solidification simulation for Al-4Mg-2Si-2Cu alloy. Part B. Simulation performed using SCHEIL module.
31	Calculations of CVM and comparisons with sublattices of a fictitious A B system. Also shows how to overlay diagrams from two calculations.
32	Calculation of oxide layers on steel. Also shows how to append databases.
33	Benchmark calculation - An isopleth in the Fe-Cr-C system.
34	Calculation of the phase diagram and G curves in the Al-Zn system. An example of using the BINARY module.
35	Calculation of potential diagram
36	<p>Assessment - The use of the PARROT module</p> <p>The example is divided into four parts corresponding to the files in the folder.</p> <p>The problem is presented with "selected" experimental data (see the <i>tcex.36.readme</i> file). The example uses a fictitious binary A-B system where element A is BCC until it melts. Element B is BCC up to 1100 K and FCC above. There is a compound A<sub>2</sub>B stable in a limited temperature range.</p> <ul style="list-style-type: none"> <li>• The creation of the "setup" file is described (<i>tcex36a.TCM</i>)</li> <li>• The creation of the experimental data file is described (<i>tcex 36b.TCM</i>)</li> <li>• The actual run in the PARROT module in order to obtain the result (<i>tcex 36cp-d.TCM</i>)</li> </ul>
37	Calculation of an isothermal section using command lines.
38	Calculation of the Morral "rose" (miscibility gaps).

#	Example Description
39	<p>This example shows how Thermo-Calc calculates the reversible Carnot cycle of a heat engine using one mole of an ideal gas with two fictitious species A and A2.</p> <p>The Reversible Carnot cycles are usually drawn schematically. Using Thermo-Calc and realistic data it is possible to calculate a reversible Carnot cycle of a heat engine and to relate it to different thermodynamic quantities.</p> <p>One application of the Second Law is to the efficiencies of heat engines, pumps and refrigerators. Whenever there is a difference of temperature, work can be produced - the principle of heat engines. The Gibbs energy also enables the prediction of the maximum work that a process may achieve.</p>
40	<p>A series of examples designed to demonstrate the advanced POURBAIX module calculations and graphical processing. Also see the text file the Extended folder (<i>TCEX40-README.txt</i>).</p> <p>The first example automatically calculates and plots a Pourbaix diagram for 0.001 m Fe in a 0.1 m NaCl aqueous solution at 25C and 1 bar. A so-called Pourbaix diagram is actually a phase diagram with independently-varied acidity (pH) and electropotential (Eh), for a heterogeneous interaction system at a certain bulk composition (that is by default always set as 1 kg of water dissolving a specified amount of metals and other solutes), under a defined temperature and pressure condition.</p> <p> For details about the other examples, see <a href="#">Pourbaix Examples TCEX40, 40A to 40E, and TCEX53</a> on page 168.</p>
41	Calculation of a solubility product. Shows the STEP_WITH_OPTION command, T-ZERO option.
42	Formation of para-pearlite (isopleth calculation) Fe-Mn-C system at 2.5%Mn Mass u-fraction (an example of a paraequilibrium calculation).
43	Formation of para-pearlite (calculation of isothermal section) Fe-Mn-C system at 700 C (an example of a paraequilibrium calculation).
44	This example uses variables and functions to predict properties e.g. proof strength for an austenitic stainless steel at elevated temperatures (20-550C).
45	<p>3D-diagram that calculates the gamma volume in the Fe-Cr-C system.</p> <p>To view the generated file, <i>tcex45.wrl</i>, install a WRML (Wirtual Reality Modelling Language) viewer to the web browser. WRML viewers can be downloaded from various sites, e.g. <a href="http://www.parallelgraphics.com">www.parallelgraphics.com</a> or <a href="http://www.sim.no">www.sim.no</a>.</p>
46	<p>3D-diagram that calculates the liquidus surface of the Fe-Cr-C system.</p> <p>To view the generated file, <i>tcex46_tri.wrl</i> and <i>tcex46_sqrt</i>, install a WRML (Wirtual Reality Modelling Language) viewer to the web browser. WRML viewers can be downloaded from various sites, e.g. <a href="http://www.parallelgraphics.com">www.parallelgraphics.com</a> or <a href="http://www.sim.no">www.sim.no</a>.</p>

#	Example Description
47	3D-quaternary diagram that calculates the gamma volume in the Fe-Cr-V-C system at 1373K. To view the generated file, <i>tcex47.wrl</i> , install a VRML (Virtual Reality Modelling Language) viewer to the web browser. VRML viewers can be downloaded from various sites, e.g. <a href="http://www.parallelgraphics.com">www.parallelgraphics.com</a> or <a href="http://www.sim.no">www.sim.no</a> .
48	This is an example of Scheil solidification with C back diffusion in solid phases and compares it with simple Scheil and equilibrium calculations.
49	This example shows how to enter parameters for a FACT quasichemical liquid model and how to calculate the sulfur activity using the GIBBS_ENERGY_SYSTEM (GES) module commands.
50	This example shows the quasichemical model using TDB to replicate figures 3 and 4 from Kongoli, F., Pelton, A. D. & Dessureault, Y. Thermodynamic modeling of liquid Fe-Ni-Cu-Co-S mattes. <i>Metall. Mater. Trans. B</i> 29, 591–601 (1998).
51	Calculation of molar volume, thermal expansivity and density.
52	This example shows how to change the excess models for binary/ternary interactions in a solution phase, either through direct interactive amendments of phase descriptions within the GIBBS_ENERGY_SYSTEM (GES) module, or enforced by specific type-definitions given in a database file retrieved by the TDB module. For binary excess model: from the default R-K model to Mixed-Excess-Model (Note the phase has to be a substitutional phase) For Ternary Extrapolation Model: from the default R-K-M model to Toop_Kohler model.
53	Pourbaix Diagram Calculations through the TDB-GES-POLY-POST routine. Using PAQ2 or PAQS2 database; for the Fe-X-H <sub>2</sub> O-NaCl heterogeneous interaction systems (X = Cr-Ni-Co).

## The Thermo-Calc Modules and Activities



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



For the Console Mode only commands see [The Console Mode Interface on page 111](#) and the *Thermo-Calc Console Mode Command Reference* included with this documentation set.

**Modules and Activities** briefly describes the available modules. The specific modules, using the names in the table, are accessed through Console Mode. For Graphical Mode, the underlying principles, and the

final calculations, are incorporated into the projects and activities. Some modules require additional licenses.

## Modules and Activities

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

Full Module Name in Console Mode	Short Name	Graphical Mode Activity	Primary Functions
BINARY_DIAGRAM_EASY	<a href="#">BIN</a>	<i>Binary Calculator on page 104</i>	Calculate binary phase diagrams. Access to specific databases designed for BIN, such as TCBIN, is required.
DATABASE_RETRIEVAL	<a href="#">DATA</a>	<i>System Definer on page 54</i>	Select appropriate databases, define chemical systems and retrieve the data required for calculations.
DICTRA_MONITOR	DICTRA	Console Mode only	Run simulations of diffusion controlled transformations in Thermo-Calc using the Diffusion Module (DICTRA). An additional license is required for this feature.
DIC_PARROT	DIC_PARROT	Console Mode only	This is the data optimization module for the Diffusion Module (DICTRA). It allows you to assess experimental data and use such data to optimize calculations. An additional license is required for this feature.
EDIT_EXPERIMENTS	<a href="#">ED_EXP</a>	Console Mode only	Part of the PARROT submodule, use it to edit experimental data points to make reliable optimizations.
GIBBS_ENERGY_SYSTEM	<a href="#">GIBBS</a>	Console Mode only	Handles thermodynamic models and quantities. Generally you do not need to use this module, but you can get information about models, and list, add or amend the thermodynamic parameters in use.
PARROT	<a href="#">PARROT</a>	Console Mode only	A data optimization module to assess experimental data and use the data to optimize calculations.
not available	-	<i>Precipitation Calculator on page 78</i>	Set the conditions for, and perform, a precipitation calculation.

Full Module Name in Console Mode	Short Name	Graphical Mode Activity	Primary Functions
not available	-	<i>Property Model Calculator</i> on page 60	You can evaluate models simultaneously over a range of compositions and cross plot the results. You can then conduct an uncertainty analysis and plot the results as either a histogram or as a probability plot.
POLY-3	<a href="#">POLY</a>	<i>Equilibrium Calculator</i> on page 72	Equilibrium calculation module. Specify conditions and make calculations.
POST_PROCESSOR	<a href="#">POST</a>	<i>Plot Renderer</i> on page 83	For post-processing and plotting of calculation results. Modify property and phase diagrams, add labels, change the diagram colours, etc. Submodules to POLY-3 and DICTRA module for example.
POTENTIAL_DIAGRAM	<a href="#">POTENTIAL</a>	<i>Ternary Calculator</i> on page 106	Calculate and plot gas potential diagrams in a ternary system. The potential of two gas species are used as the diagram axes.
POURBAIX_DIAGRAM	<a href="#">POURBAIX</a>	Console Mode only	Calculate and plot pH-Eh diagrams (Pourbaix diagrams) and property diagrams for heterogeneous interaction systems involving aqueous solutions.
REACTOR_SIMULATOR_3	<a href="#">REACTOR</a>	Console Mode only	Simulate chemical reaction processes in several feed-forward steady-state stages or in several dynamic stages.
SCHEIL_SIMULATION	<a href="#">SCHEIL</a>	<i>Scheil Calculator</i> on page 108	Simulate and plot Scheil-Gulliver solidification processes with no diffusion in the solid phases and with/without consideration of back diffusion of interstitial components (such as C, N, O, S).
SYSTEM_UTILITIES	<a href="#">SYS</a>	Console Mode only	In Console Mode, interact with the operating system and change environmental settings. Create and execute MACRO files.
TABULATE_REACTION	<a href="#">TAB</a>	Console Mode only	Tabulate properties of chemical reactions and substances (stoichiometric or solution phases).

Full Module Name in Console Mode	Short Name	Graphical Mode Activity	Primary Functions
TERNARY_DIAGRAM	<a href="#">TERN</a>	<i>Ternary Calculator</i> on page 106	Calculate ternary phase diagrams.

## Displaying Thermo-Calc License Information

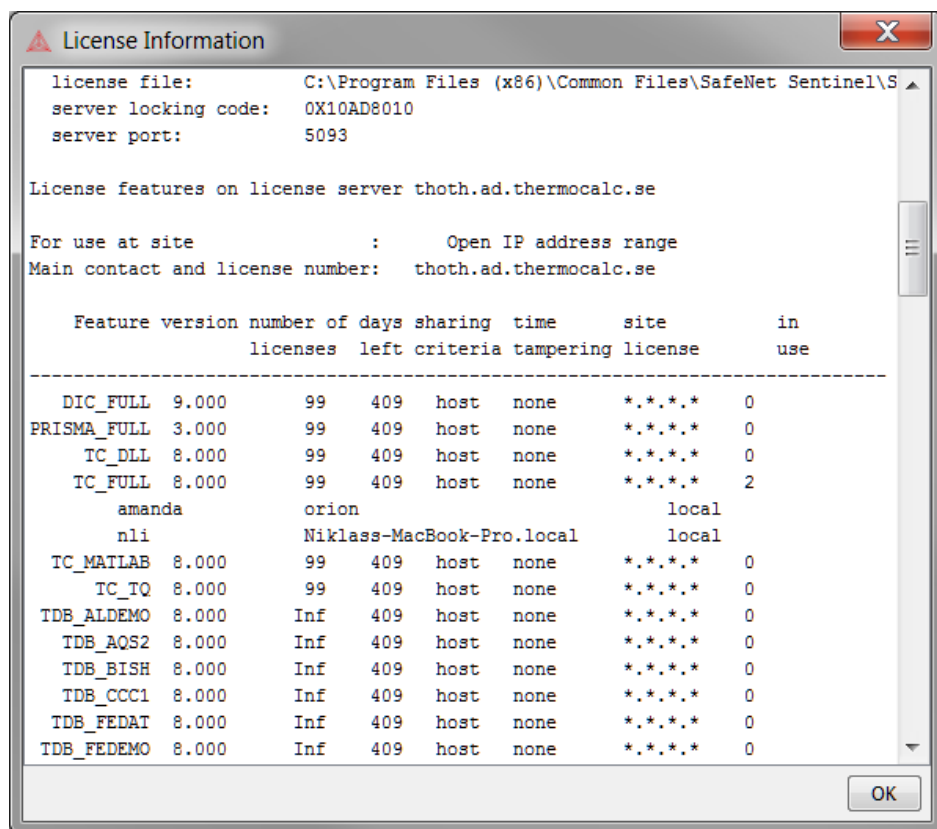
You can start (and install) the software without a valid Thermo-Calc license but you cannot do any calculations. To show information about the available and installed licenses, from the main menu select **Help → Show License Info**.



Also see the *Thermo-Calc Installation Guide*.

### License Information Window Example

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



Under each license type with instances checked out, there is a list of who checked out each license. In Graphical Mode, an instance is checked out when an Equilibrium Calculator activity is created, and

checked back in when that Equilibrium Calculator is removed. In Console Mode, an instance is checked out when you enter the POLY module and is checked back in when you exit the POLY module. In the example, two users, amanda and nli, have licenses checked out.

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

### Console Mode License Restrictions

- If you start Thermo-Calc without a valid Thermo-Calc license you cannot leave the SYS module.
- If all the licenses are checked out for a network client installation of Thermo-Calc, you may not be able to enter the POLY or DICTRA modules until a license is available.
- To enter the DICTRA and the DIC\_PARROT modules, you need a valid Diffusion Module (DICTRA) license key.
- If you enter and use either the DIC\_PARROT module or the PARROT module, then you cannot enter the other module in the same session. You must close down Thermo-Calc and launch the program again to enter the other data optimization module.

### Network Computer License Restriction

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

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

## Using This Guide

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



Additional documentation and training material is described in [Help Resources on page 5](#).

### Graphical Mode

[The Graphical Mode Interface on page 26](#) introduces you to the GUI layout and the workflow. In [Graphical Mode Projects on page 42](#), it goes into more detail about how to set up and run your projects (with the Quick Start Wizard), using templates, scheduling jobs and creating activities. [Graphical Mode Activities on page 53](#) specifically describes how to set up each type of available activity in the tree structure.

For both Graphical and Console mode, [Changing Global Settings on page 187](#) gives information about adjusting global user settings.

## Console Mode

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

In this guide it is a basic introduction to the layout of the Command windows, as described in [The Console Mode Interface on page 111](#).

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

- [Equilibrium Calculations on page 130](#)
- [Property Diagrams on page 136](#)
- [Phase Diagrams on page 140](#)
- [Scheil Simulations on page 144](#)
- [T<sub>0</sub> Temperature Simulations on page 150](#)
- [Paraequilibrium on page 153](#)
- [Potential Diagrams on page 157](#)
- [Aqueous Solutions on page 161](#)
- [Console Mode TAB Module on page 174](#)

Then in [Console Mode POST Module on page 179](#) there is an overview of plotting.

For both Graphical and Console mode, [Changing Global Settings on page 187](#) gives information about adjusting global user settings.



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# The Graphical Mode Interface

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

In this section:

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<i>The GUI Layout</i> .....	27
<i>Project Activities and the Tree Structure</i> .....	28
<i>Activity Successor and Predecessor Nodes</i> .....	28
<i>Creating Activities and Successors</i> .....	29
<i>Graphical Mode Workflow</i> .....	31
<i>Main Menu and Toolbar</i> .....	32
<i>Saving and Opening Thermo-Calc Project Files</i> .....	34
<i>Project Activity Nodes</i> .....	34
<i>Project and Activity Menus</i> .....	36
<i>Moving Windows</i> .....	38
<i>Moving Nodes in the Tree and Using the Grid</i> .....	39
<i>Node Status Markers</i> .....	40

## The GUI Layout

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



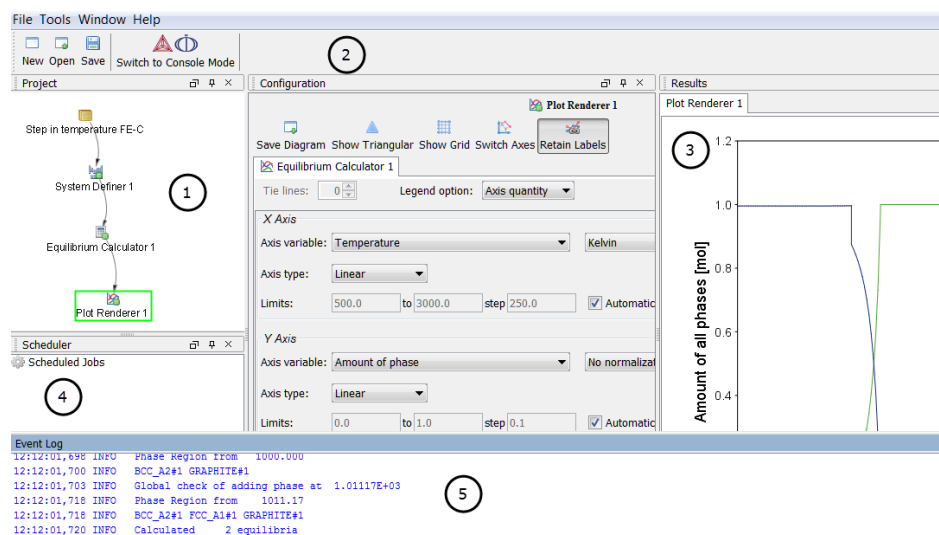
Also see [Moving Windows](#) on page 38.

The windows are:

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

### Graphical Mode Windows

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



## Project Activities and the Tree Structure

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



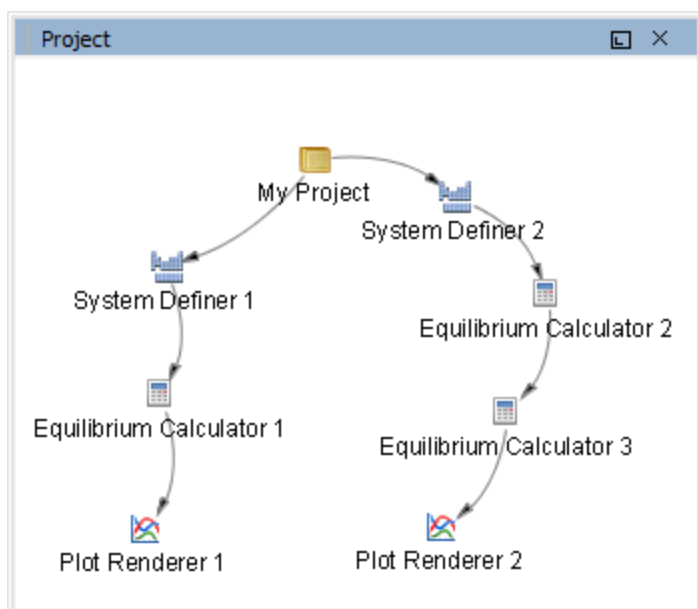
Also see [Activity Successor and Predecessor Nodes](#) below for definitions.

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

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

### Project Tree Example

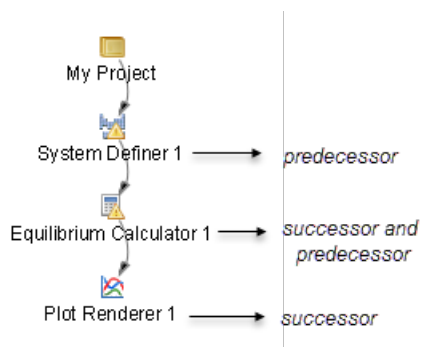
Project window with a My Project node. There are two trees with successor and predecessor activity nodes.



## Activity Successor and Predecessor Nodes

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

### Example of the Tree Structure



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

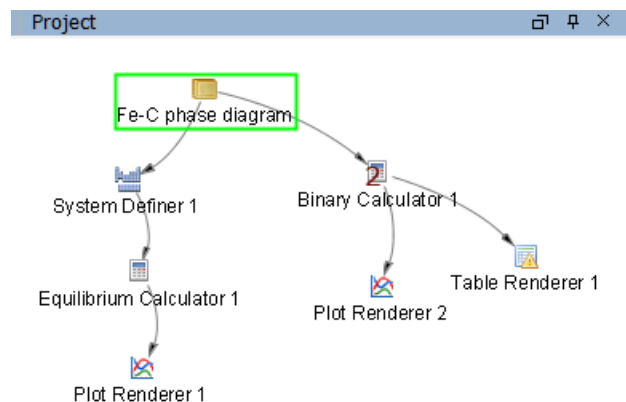
See [Successor and Predecessor Example below](#), which shows that Binary Calculator 1 is a predecessor to the successors, Plot Renderer 2 and Table Render 1.

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



Also see [Creating Activities and Successors below](#).

### Successor and Predecessor Example



## Creating Activities and Successors

You can create a new activity in these ways:

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

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

## Predecessors and Successors by Activity

Activity	Possible Predecessors	Possible Successors
My Project	None; this is the first node of the tree structure	System Definer, Binary Calculator, Ternary Calculator, Experimental File Reader. Also choose templates from this level.
<a href="#">System Definer on page 54</a>	My Project, System Definer	Property Model Calculator, Equilibrium Calculator, Precipitation Calculator, Scheil Calculator
<a href="#">Property Model Calculator on page 60</a>	System Definer	Plot Renderer
<a href="#">Equilibrium Calculator on page 72</a>	System Definer, Equilibrium Calculator	Equilibrium Calculator, Plot Renderer, Table Renderer
<a href="#">Precipitation Calculator on page 78</a>	System Definer	Plot Renderer, Table Renderer
<a href="#">Plot Renderer on page 83</a>	Property Model Calculator, Equilibrium Calculator, Precipitation Calculator, Binary Calculator, Ternary Calculator, Scheil Calculator, Experimental File Reader	None
<a href="#">Table Renderer on page 101</a>	Equilibrium Calculator, Precipitation Calculator, Binary Calculator, Scheil Calculator	None
<a href="#">Experimental File Reader on page 104</a>	My Project	Plot Renderer
<a href="#">Binary Calculator on page 104</a>	My Project	Plot Renderer, Table Renderer
<a href="#">Ternary Calculator on page 106</a>	My Project	Plot Renderer
<a href="#">Scheil Calculator on page 108</a>	System Definer	Plot Renderer, Table Renderer

## Graphical Mode Workflow

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

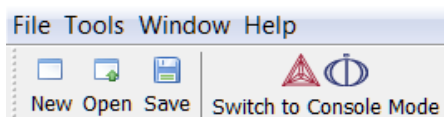
The typical workflow is to:

1. *Define a System*: Create a [System Definer on page 54](#) activity (in the **Project** window) where you select a database and the elements to have as system components (in the **Configuration** window).
2. *Set up and run a calculation*: Create an [Equilibrium Calculator on page 72](#) activity (a successor to the **System Definer**), where calculation conditions are set (temperature, pressure, etc.). This is where axis variables are set to create a property or phase diagram. These settings are also made in the **Configuration** window. You can also create a [Property Model Calculator on page 60](#), [Precipitation Calculator on page 78](#) or [Scheil Calculator on page 108](#).
3. *Visualize the results*: Create either a [Plot Renderer on page 83](#) or a [Table Renderer on page 101](#) activity in the **Project** window. When calculated, this creates a plot or table in the **Results** window. The results are shown in a **Plot Renderer** or a **Table Renderer** tab.



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

## Main Menu and Toolbar



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




In Console Mode you use commands to access the other options instead. These are discussed in [The Console Mode Interface on page 111](#).

### Graphical Mode Menu and Toolbar Options

Option	Description	Action (s)
New	Create a new project.	Click <b>New</b> on the toolbar Select <b>File → New Project</b> Press <Ctrl+N>
Open	Open an existing project. See <a href="#">Saving and Opening Thermo-Calc Project Files on page 34</a> .	Click <b>Open</b> on the toolbar Select <b>File → Open Project</b>

Option	Description	Action (s)
		Press <Ctrl+O>.
Save	Save a project. See <a href="#">Saving and Opening Thermo-Calc Project Files on the next page</a> .	Click <b>Save</b> on the toolbar Select <b>File → Save Project</b> Press <Ctrl+S>.
Switch to Console Mode	Launch Console Mode and the command prompt.	Click the button to exit Graphical Mode and open Console Mode.
Switch to Graphical Mode	Launch Graphical Mode to work with the GUI version.	Click the button to exit Console Mode and open Graphical Mode.
Append Project	Combine two projects into one project file. See <a href="#">Saving and Opening Thermo-Calc Project Files on the next page</a> .	Select <b>File → Append Project</b>
Save Project As...	Save an existing project with a new name.	Select <b>File → Save Project As...</b>
Exit	Exit the program.	In the upper right-corner of the program, click the X. Select <b>File → Exit</b> Press <Ctrl+Q>.
Options	Change the global defaults for a variety of settings. See <a href="#">Changing Global Settings on page 187</a> .	Select <b>Tools → Options</b>
Database Checker	Open the Database Checker, a program to check that the syntax of Thermo-Calc database files is correct. This is for advanced users who develop and manage databases.	Select <b>Tools → Database Checker</b>
Window menu	Highlight a specific window on the GUI	From the <b>Window</b> menu, select an option to refocus on that specific window.
Online Help	Open the online help system where you can browse or search all the Thermo-Calc documentation.	Select <b>Help → Online Help</b>
Show License Info	Open the License Information window.	Select <b>Help → Show License Info</b>



Option	Description	Action (s)
	 Also see <a href="#">Displaying Thermo-Calc License Information on page 23</a> and in the <i>Thermo-Calc Installation Guide</i> .	
Check for update	Check the Thermo-Calc Software website for updates to the software.	Select <b>Help</b> → <b>Check for update</b>

## Saving and Opening Thermo-Calc Project Files

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

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

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

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



Also see [Saving Plots on page 95](#) and [Saving Tabulated Data for the Table Renderer on page 101](#).


## Project Activity Nodes

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

### Project Activity Node Descriptions

These are the project activity nodes available in Graphical Mode.

Activity type	Description
<a href="#">System Definer on page 54</a>	Define a certain thermodynamic system and read it from file into memory.
<a href="#">Property Model Calculator on page 60</a>	Choose one or more general models to predict and optimize material properties. You can evaluate models simultaneously over a range of compositions and cross plot the results. You can then conduct an uncertainty analysis and plot the results as either a histogram or as a probability plot.
<a href="#">Equilibrium Calculator on page 72</a>	Set thermodynamic conditions and define axis variables when a series of equilibrium calculations are to be performed in one or more dimensions.
<a href="#">Precipitation Calculator on page 78</a>	Set the conditions for, and perform, a precipitation calculation.
<a href="#">Plot Renderer on page 83</a>	Determine the layout of non-text based output.
<a href="#">Table Renderer on page 101</a>	Use it for text-based output.
<a href="#">Binary Calculator on page 104</a>	<p>Use it for some calculations involving two components only. It is like a combination of System Definer and Equilibrium Calculator activities with adaptations to simplify the configuration of calculations on binary systems.</p> <p> To perform this activity, you need a database designed for the Binary Calculator, such as the TCBIN database.</p>
<a href="#">Ternary Calculator on page 106</a>	<p>Use it for some calculations involving three components. It is like a combination of System Definer and Equilibrium Calculator activities with adaptations to simplify the configuration of calculations on ternary systems.</p> <p> To get a reliable result you need a database that fully assesses binary and ternary systems.</p>
<a href="#">Scheil Calculator on page 108</a>	Perform Scheil-Gulliver calculations (also known as Scheil calculations). A default Scheil calculation is used to estimate the solidification range of an alloy assuming that i) the liquid phase is homogeneous at all times and ii) the diffusivity is zero in the solid. However, it is possible to disregard the second assumption for selected components.
<a href="#">Experimental File Reader on page 104</a>	Read experimental data files (*.EXP). This type of file contains information specifying a plotted diagram, written in the DATAPLOT graphical language.

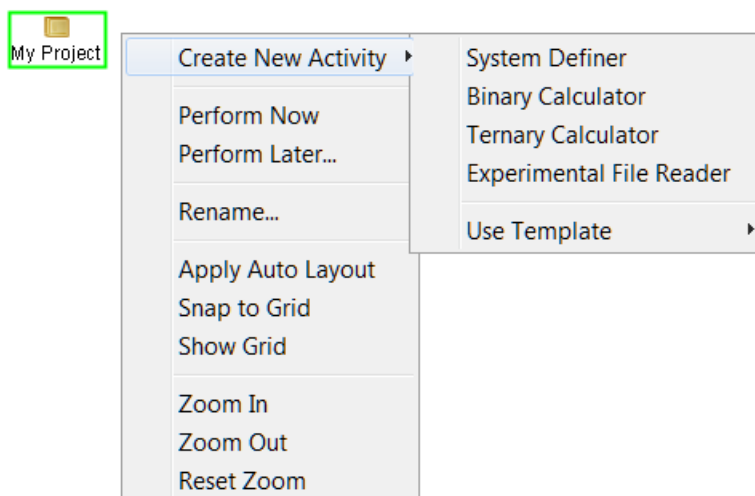
Activity type	Description
	 Also see the <i>DATPLOT User Guide</i> .

## Project and Activity Menus

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

### My Project Node

Menu options available for My Project node.



### Activity Node Menu Example

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

Create New Successor	Property Model Calculation
Perform Now	Equilibrium Calculator
Perform Later...	Scheil Calculator
Perform Tree Now	Precipitation Calculator
Perform Tree Later...	
Rename...	
Remove	
Clone	
Clone Tree	
Apply Auto Layout	
Snap to Grid	
Show Grid	

### Menu Options for Activities

Option	Description	Action (s)
Create New Activity	Add System Definer, Binary Calculator, Ternary Calculator, and Experimental File Reader nodes. <i>See <a href="#">Creating Activities and Successors</a> on page 29.</i>	Right-click <b>My Project</b> and from the <b>Create New Activity</b> menu choose an option.
Create New Activity → Use Template	Choose from the available templates to use the Wizard or add predefined nodes. <i>See <a href="#">Creating a Project from a Template</a> on page 46.</i>	Right-click <b>My Project</b> and from the <b>Create New Activity</b> → <b>Use Templates</b> menu choose an option.  The templates are also available on the <b>Configuration</b> window, which you can access by clicking the <b>My Project</b> node, or from the <b>Window</b> menu.
Create New Successor	Add a successor to the selected node. <i>See <a href="#">Creating Activities and Successors</a> on page 29.</i>	Right-click one of these nodes <b>System Definer, Property Model Calculator, Equilibrium Calculator, PRISM Calculator, Binary Calculator, Ternary Calculator</b> or <b>Experimental File Reader</b> , and from the <b>Create New Successor</b> menu choose an option.

Option	Description	Action (s)
Add a Predecessor	Add a predecessor to the selected node.	Right-click a node to add a predecessor to it (when available).
Perform Now or Perform Later	Perform a calculation or create a plot or table immediately, or schedule it for a time in the future. See <a href="#">Using the Scheduler on page 49</a> .	Right-click any node.
Rename	Change the name of the node.	Right-click any node.
Remove	Delete the selected node from the tree.	Right-click any node except My Project.
Clone	Duplicate the selected node and add it to the same tree. See <a href="#">Cloning Activities and Trees on page 47</a> .	Right-click any node except My Project.
Clone tree	Duplicate a tree and add it to My project.	Right-click any node except My Project.
Apply Auto Layout	Apply an automatic layout to the nodes in the tree.	Right-click any node.
Snap to Grid	Snap a node to align it with the grid. See <a href="#">Moving Nodes in the Tree and Using the Grid on the next page</a> .	Right-click any node.
Show Grid	Turn the grid on or off in the Project window.	Right-click any node.
Zoom In, Zoom Out, Reset Zoom	Zoom in and out of the Project window or reset the zoom to the default.	Right-click any node.

## Moving Windows

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








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

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

### Floating, Hiding and Minimizing Windows in the GUI

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

listed in the table.

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

## Moving Nodes in the Tree and Using the Grid

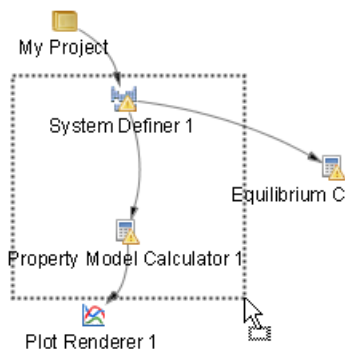
In the Project window, you can work with the activity nodes in these ways.

### Select and Move Individual Nodes

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

### Select Several Nodes at a Time

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



### Zoom In and Out

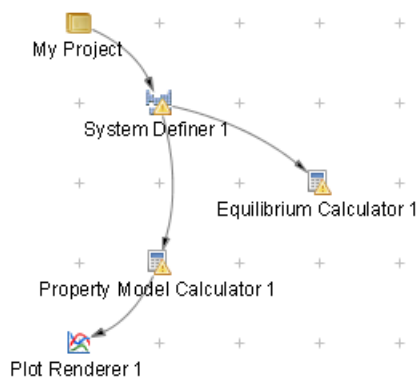
- Zoom in and out with the mouse scroll wheel.
- In the **Project** window right-click and select **Zoom In** or **Zoom Out**. To go back to the default zoom, select **Reset Zoom**.

### Show Grid and Snap to Grid

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

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









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



### Node Status Markers

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

#### Node Status Markers for the Project and Scheduler Windows

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



---

## Graphical Mode Projects

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

In this section:

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<i>The Quick Start Wizard .....</i>	<i>43</i>
<i>Creating a Project with the Quick Start Wizard .....</i>	<i>43</i>
<i>Creating a Project from a Template .....</i>	<i>46</i>
<i>Cloning Activities and Trees .....</i>	<i>47</i>
<i>Performing Projects, Trees and Activities .....</i>	<i>49</i>
<i>Using the Scheduler .....</i>	<i>49</i>
<i>The Event Log .....</i>	<i>51</i>

## The Quick Start Wizard

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

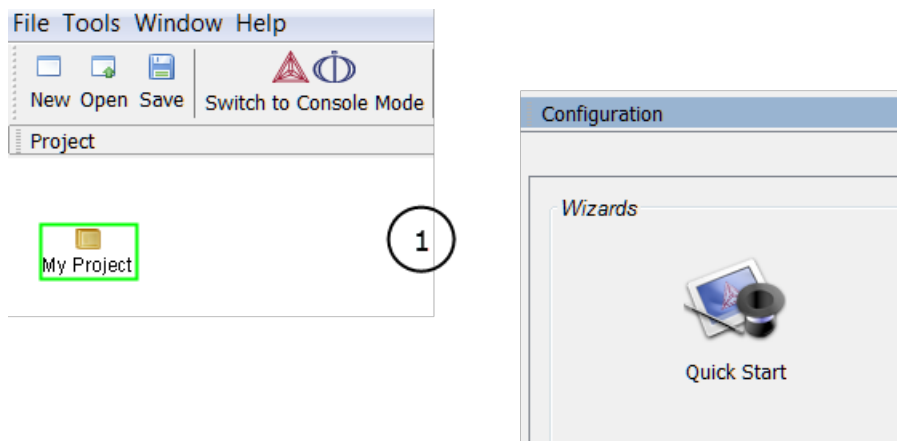
- Single point equilibrium
- Property diagram
- Phase diagram
- Scheil solidification simulation

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

## Creating a Project with the Quick Start Wizard

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

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



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

**Select Project Type**

Select the kind of calculation that you want to perform.

**Steps**

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

☒ Single point equilibrium

☐ Property diagram

☐ Phase diagram

☐ Scheil solidification simulation

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

**Define System**

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

**Steps**

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

☒ Database FEDEMO: Iron Demo Database

*Elements*

☐ C

☐ Cr

☐ Fe

☐ Mn

☐ Ni

☐ Material file  Material file

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

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

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

**Select Conditions**

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

**Steps**

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

Composition unit Mass percent

*Condition Definitions*

Temperature Kelvin 1000.0

Composition C 99.99

Composition Fe 0.01

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

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

6. Click **Finish**.

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

```

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

```

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

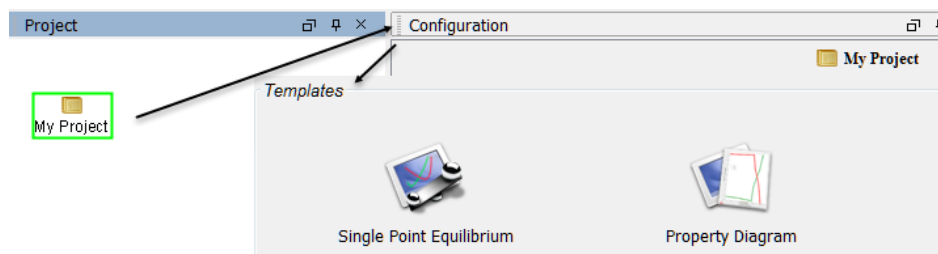
Results				
Table Renderer 1				
<b>System</b>				
Moles	1.00000			
Mass	12.01194	[g]		
Temperature	1000.00000	[K]		
Total Gibbs Energy	-12659.53136	[J]		
Enthalpy	11784.43824	[J]		
Volume	5.39784E-6	[m3]		
<i>Component</i>	<i>Mole Fraction</i>	<i>Mass Fraction</i>	<i>Activity</i>	<i>Potential</i>
Fe	0.00002	0.00010	0.00619	-42278.5054
C	0.99998	0.99990	0.21816	-12658.8942
<b>Stable Phases</b>				
	<i>Moles</i>	<i>Mass</i>	<i>Volume Fraction</i>	
BCC_A2#1	0.00002	0.00120	0.00003	Composition

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

## Creating a Project from a Template

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

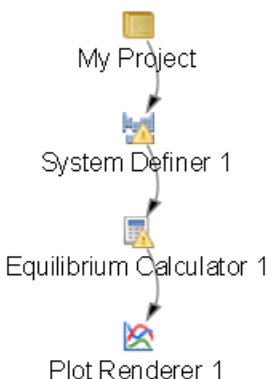
### Configuration Window Templates



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

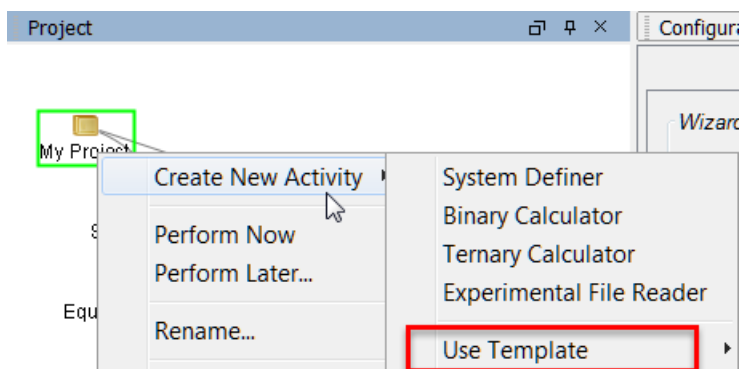
For example, if you click **Property Diagram**, a tree is added to the **My Project** node with **System Definer**, **Equilibrium Calculator** and **Plot Renderer** nodes.

### Property Diagram Template



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

### Use Template Submenu



## Cloning Activities and Trees

As described in [Creating Activities and Successors on page 29](#), you can clone a single activity or the selected activity and all the activities that come after it (successors). The predecessor of the selected activity also is the predecessor of the clone.

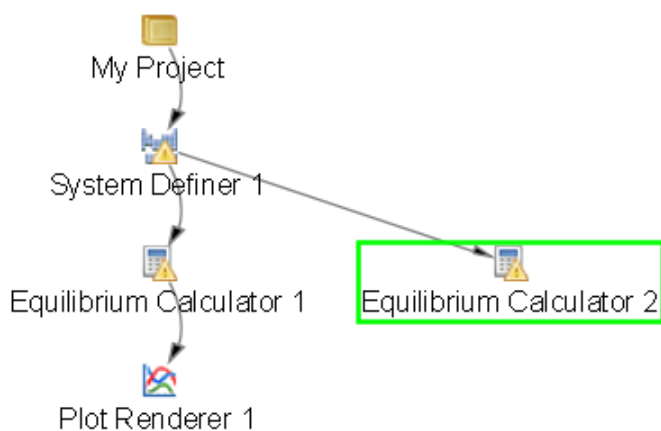
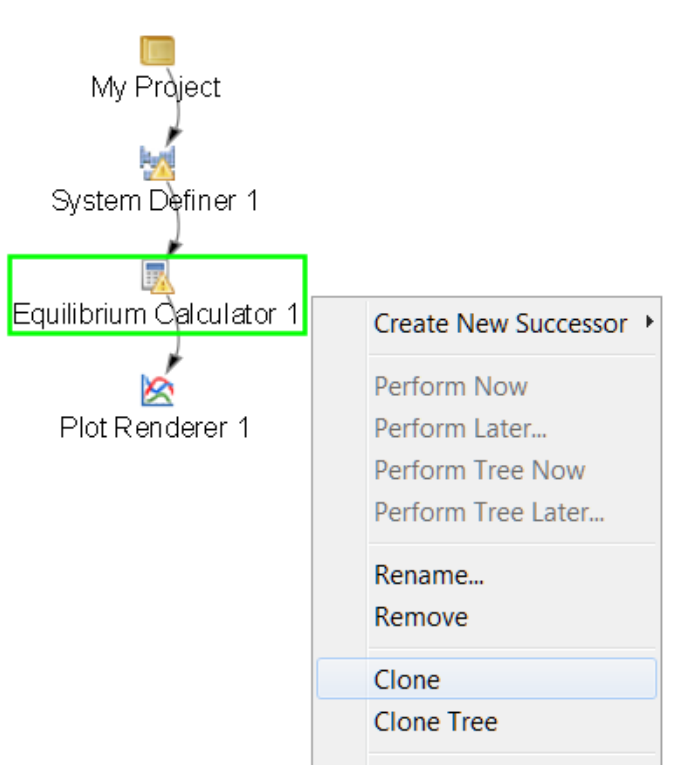
Cloned activities are configured exactly like the activities that they were cloned from, and any results of calculations or plots are also cloned. To clone a selected activity, right-click the activity and select **Clone**.

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

The following applies to clones.

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

### Cloning an Equilibrium Calculator Activity Node



### Equilibrium Calculator Clones and Successors

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



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

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

## Performing Projects, Trees and Activities

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

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



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

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

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



If there is an error during the performance of an activity, icons display status markers, which are described in [Node Status Markers on page 40](#).

## Using the Scheduler

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



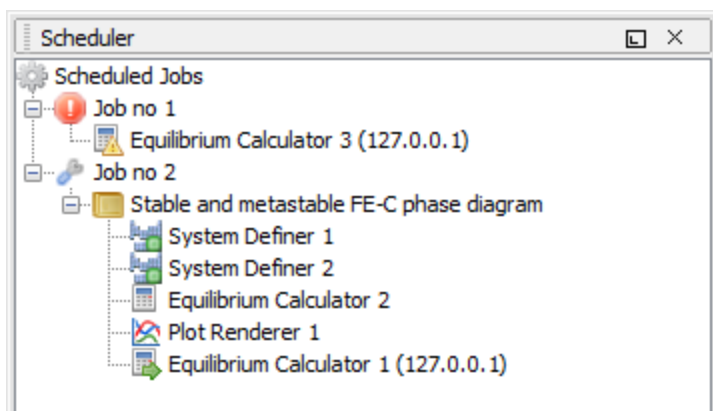
The following applies to jobs.

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



Also see [Node Status Markers](#) on page 40.

## Scheduled Jobs Example



## Managing the Schedule

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

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

## The Event Log

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

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

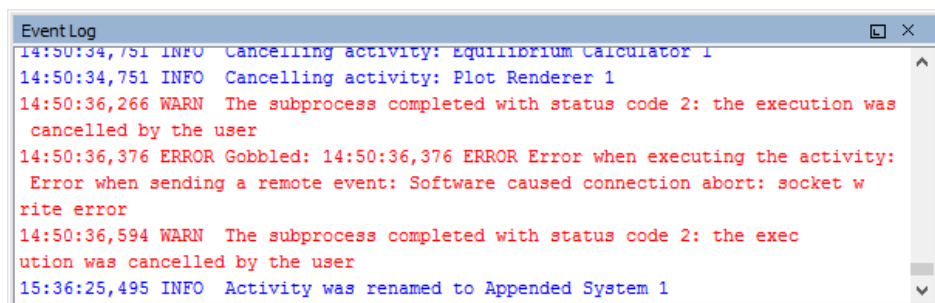
To specify the level of detail in the Event Log window, from the main menu select **Tools →Options**. In the **General** tab set the **Log level** slide bar to anything between **Debug** (most detailed) and **Error** (least detailed).



Also see [Changing Global Settings on page 187](#).

## Event Log Window Example

The example shows information, warnings and errors.



---

## Graphical Mode Activities

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

In this section:

---

<i>System Definer</i> .....	54
<i>Property Model Calculator</i> .....	60
<i>Equilibrium Calculator</i> .....	72
<i>Precipitation Calculator</i> .....	78
<i>Plot Renderer</i> .....	83
<i>Table Renderer</i> .....	101
<i>Experimental File Reader</i> .....	104
<i>Binary Calculator</i> .....	104
<i>Ternary Calculator</i> .....	106
<i>Scheil Calculator</i> .....	108

## System Definer

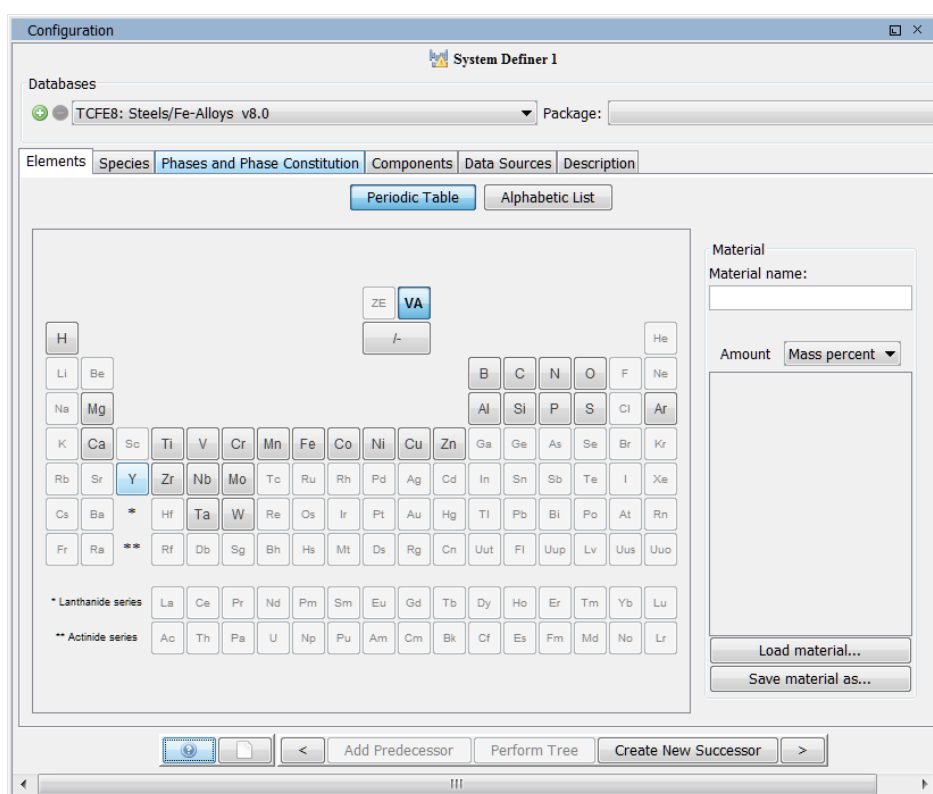
In a System Definer activity, you select the database to use to retrieve thermodynamic data and define which elements the system has as components. You can also select which species to include as well as change the reference temperature and pressure for your components.



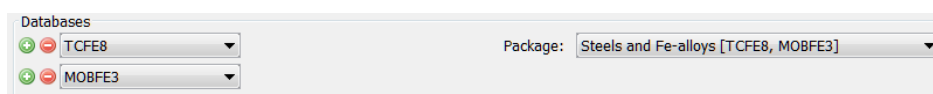
Also see [Creating Activities and Successors on page 29](#) for a list of possible successors and predecessors for this activity.

## The System Definer Settings

### Configuration Window



### Choose Database(s) or a Database Package



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

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

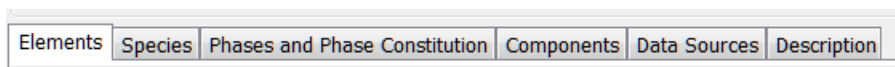


Also see [Global Settings: System Definition \(System Definer\)](#) on page 191 to learn how to create a database package.

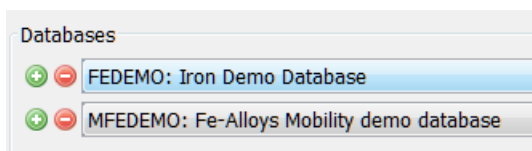


If you have chosen a database package and then remove or change a database, a message displays *Selected databases and selected package may differ*. This means that the original package you selected, which added preset databases, does not match the databases you are using for the project. For information about how to clear the message, see [Global Settings: System Definition \(System Definer\)](#) on page 191.

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



The following example uses the FEDEMO and MFEDEMO databases and Example 12 available with the [Graphical Mode Example Collection](#) on page 9.

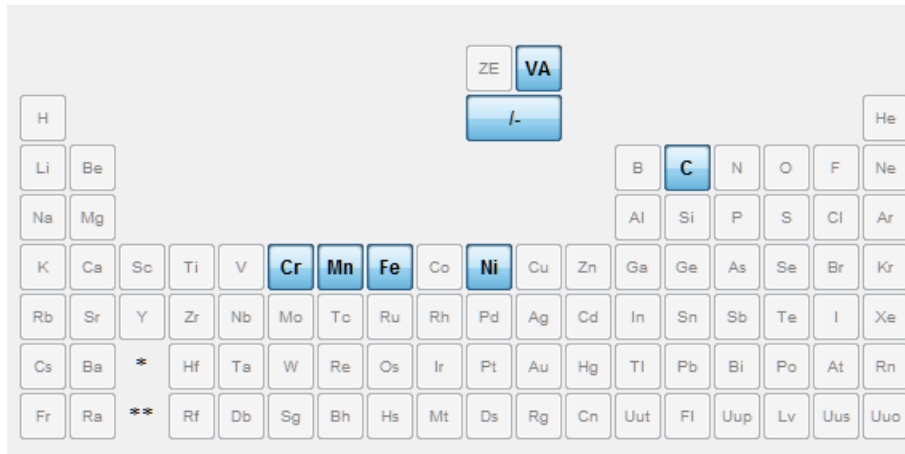


## Elements

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

## Periodic Table

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



## Alphabetic List

Element	FEDEMO	MFEDEMO
I-	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
C	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Cr	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Fe	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Mn	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Ni	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
VA	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>

## Material Composition

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

Material

Material name:

Amount Mass percent ▼

Fe	<input type="text" value="80.52"/>
Ni	<input type="text" value="1.4"/>
C	<input type="text" value="0.08"/>
Mn	<input type="text" value="1.0"/>
Cr	<input type="text" value="17.0"/>

At the bottom of the window, click **Load material** to open a material file. Click **Save material as** to save

the material you defined, for example **Ferritic**.



Also see [Global Settings: System Definition \(System Definer\)](#) on page 191 to learn how to create your own database packages.



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

## Species

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

Elements	Species	Phases and Phase Constitution	
Species	Stoichiometry	FEDEMO	MFEDMO
I-	-1	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
C	C	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Cr	Cr	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Fe	Fe	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Mn	Mn	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Ni	Ni	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
VA	VA	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
C2	C <sub>2</sub>	<input checked="" type="checkbox"/>	<input type="checkbox"/>
C3	C <sub>3</sub>	<input checked="" type="checkbox"/>	<input type="checkbox"/>
C4	C <sub>4</sub>	<input checked="" type="checkbox"/>	<input type="checkbox"/>
C5	C <sub>5</sub>	<input checked="" type="checkbox"/>	<input type="checkbox"/>
C60	C <sub>60</sub>	<input checked="" type="checkbox"/>	<input type="checkbox"/>

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

A dialog box titled "New species" with a close button (X) in the top right corner. Inside the dialog, there is a question mark icon and the text "Enter the species:". Below this text is a text input field. At the bottom of the dialog are two buttons: "OK" and "Cancel".

## Phases and Phase Constitution



Phases

Status	Name	FEDEMO	MFEDEMO
Entered	BCC_A2	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Entered	CEMENTITE	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Entered	CHI_A12	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Entered	DIAMOND_FCC_...	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Entered	FCC_A1	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Entered	FCC_A1#2	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Entered	GAS	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Entered	GRAPHITE	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Entered	HCP_A3	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Entered	KSI_CARBIDE	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Entered	LAVES_PHASE_...	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Entered	LIQUID	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Entered	M23C6	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Entered	M3C2	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Entered	M5C2	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Entered	M7C3	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Entered	SIGMA	<input checked="" type="checkbox"/>	<input type="checkbox"/>

☒ Check/uncheck all

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

To review the **Phase constitution** for a specific phase, click it in the **Phase** list (for example **BCC\_A2**) and its details are displayed at the bottom of the window. Click **Edit** then click an element to select or reject a constituent. The last remaining constituent on a sublattice cannot be rejected.

FEDEMO MFEDEMO

Phase BCC\_A2

**Phase constitution for current system**

(     )<sub>1.0</sub> (   )<sub>3.0</sub>

**Phase description in database**

(Cr,Fe,Mn,Ni)<sub>1</sub> (C,VA)<sub>3</sub>

## Components

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

Elements	Species	Phases and Phase Constitution	Components	Data Sources	Description
Component	Reference phase	Reference temperature	Reference pressure		
		Kelvin	Pascal		
Fe	<input checked="" type="checkbox"/> SER HCP_A3	<input checked="" type="checkbox"/> Current temperature	25.0	100000.0	
Cr	<input checked="" type="checkbox"/> SER	<input checked="" type="checkbox"/> Current temperature	25.0	100000.0	
Ni	<input checked="" type="checkbox"/> SER	<input checked="" type="checkbox"/> Current temperature	25.0	100000.0	
C	<input checked="" type="checkbox"/> SER	<input checked="" type="checkbox"/> Current temperature	25.0	100000.0	
Mn	<input checked="" type="checkbox"/> SER	<input checked="" type="checkbox"/> Current temperature	25.0	100000.0	

## Data Sources

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

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

## Description

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

Elements	Species	Phases and Phase Constitution	Components	Data Sources	Description
FEDEMO	MFEDMO				
MFEDMO - Database for Demo Version of Thermo-Calc ***** [Version 1.0: released Nov 2015] Ownership/Copyright: 2015 @ Thermo-Calc Software AB All rights reserved. MFEDMO is a kinetic database containing mobility data for Fe-based alloys.					

## Creating a System Definer Activity

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




To change the default database or create a database package, see [Global Settings: System Definition \(System Definer\)](#) on page 191.



Also see [About the Database Files](#) on page 184.

1. Right-click **My Project** and from the menu select **Create New Activity→ System Definer** .
2. In the **Project** window, click the [System Definer on page 54](#) activity node.
3. In the **Configuration** window, from the **Databases** menu choose **Database(s)** or a **Data-base Package**.

Options are to:

- Select **<User database>** to define your own.
  - You can choose to add one or more databases by clicking the **Add a database**  button.
  - From the **Package** list, choose a predefined database package to add multiple databases at a time. Depending on your license, there are predefined database packages available to select.
4. Select the **Elements** tab to choose the elements in the **Periodic Table** or use the **Alphabetic List** to choose elements for the system.
  5. As required click the tabs to make edits: **Species**, **Phases** and **Phase Constitution**, and **Components**. The **Data Sources** and **Description** tabs provide information based on the database.
  6. Click **Perform** to start the System Definer activity immediately and retrieve thermodynamic data about the system. Click the **Event Log** window to watch the progress of the job.

## Property Model Calculator

A Property Model Calculator allows you to predict and optimize material properties. A set of general models is available to use: a [Phase Transition Model on page 68](#), [Driving Force Model on page 69](#), [Interfacial Energy Model on page 70](#), [Coarsening Model on page 70](#), and an [Equilibrium Model on page 72](#).

You can evaluate models simultaneously over a range of compositions and cross plot the results. You can then conduct an uncertainty analysis and plot the results as either a histogram or as a probability plot. The **Configuration** window for a Property Model Calculator using the *Phase transition* model is shown and described in [Defining the Property Model Calculator on page 64](#).

---

## Property Model Calculator Workflow

When a project is first being designed, it is recommended you test it by first performing a **Single** calculation type. This verifies that the configuration of the model is valid, otherwise you will get a *Not a Number* result in [Event Log Window on page 116](#) window indicating the calculation did not work correctly.

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

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



Also see [The Quick Start Wizard on page 43](#) and [Creating a Project from a Template on page 46](#).



For examples using the Property Model Calculator, see examples 10, 11, and 12 in [Graphical Mode Example Collection on page 9](#).

## Configuration Window

## Configuration Settings

Setting/Button	Description
----------------	-------------

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

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

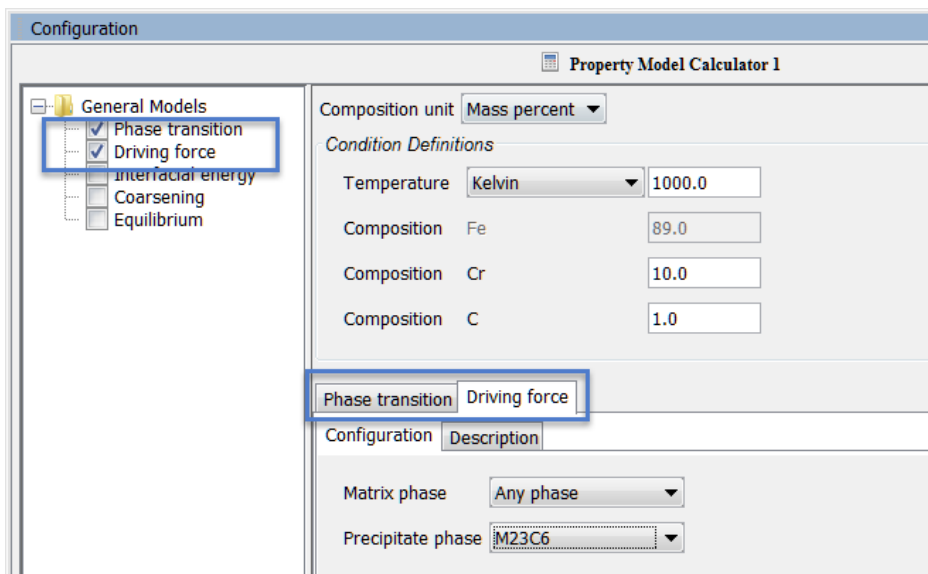


Also see [About the Uncertainty Calculations on the next page](#) for more detail.

## Defining the Property Model Calculator

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

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



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

- [Phase Transition Model on page 68](#)
- [Driving Force Model on page 69](#)
- [Interfacial Energy Model on page 70](#)
- [Coarsening Model on page 70](#)
- [Equilibrium Model on page 72](#)

## About the Uncertainty Calculations

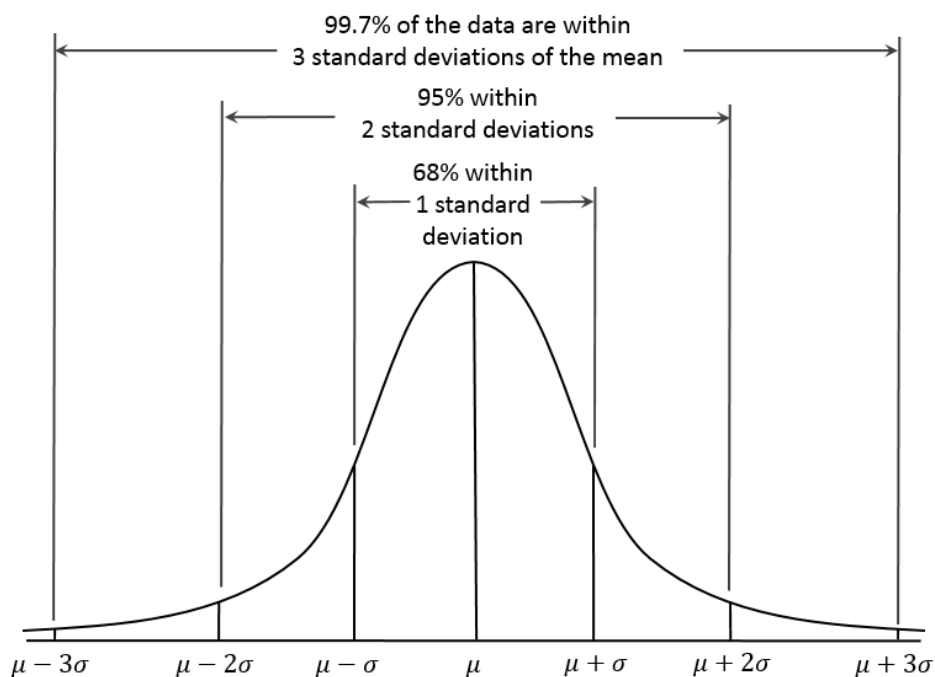
The following example uses the [Phase Transition Model on page 68](#) and an **Uncertainty Calculation Type** to describe how the sampling of data is performed. The example (which is example 10 in [Graphical Mode Example Collection on page 9](#)) predicts the transition temperature to the unwanted brittle Sigma phase and shows how the temperature is influenced by changes to a steel alloy's composition.

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

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

### Gaussian Distribution, the 3-Sigma Rule

Image by Dan Kernler, [https://en.wikipedia.org/wiki/Normal\\_distribution#/media/File:Empirical\\_Rule.PNG](https://en.wikipedia.org/wiki/Normal_distribution#/media/File:Empirical_Rule.PNG)



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

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

### Condition Definitions and Sampling Settings

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



Composition unit Mass percent

**Condition Definitions**

Temperature Celsius 600.0

Composition Fe 80.52

Composition Ni 1.4

Composition C 0.08

Composition Mn 1.0

Composition Cr 17.0

**Sampling of Data from Gaussian Distributions**

Quantity	Mean	$\Delta$ Min/Max
<input type="checkbox"/> Temperature	600.0	0.0
<input checked="" type="checkbox"/> Mass percent Ni	1.4	0.4
<input checked="" type="checkbox"/> Mass percent C	0.08	0.02
<input checked="" type="checkbox"/> Mass percent Mn	1.0	0.3

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

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

### Sampling Parameter Settings

**Sampling Parameters**

Truncate distribution at 3 standard deviations

Total number of samples 200

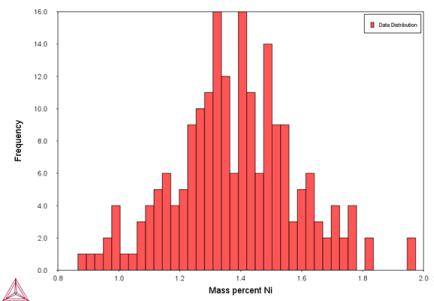
You can experiment by varying the conditions and the number of samples to see the distribution results smooth out as is to be expected based on the Central Limit Theorem. For example, on the **Plot Renderer** the variable is set to measure the **Composition of Ni**. The initial sample size uses the default,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

### Histogram Plot

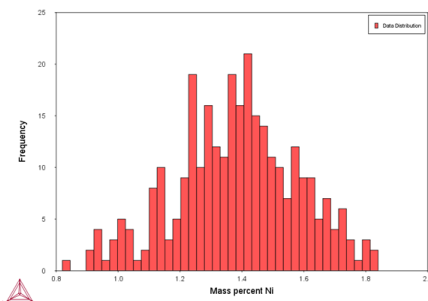
This is a series of histogram plots of the uncertainty calculations sampling data from Gaussian distributions. It compares the Ni composition where the total sample size is increased to show how the

model follows the Gauss distribution.

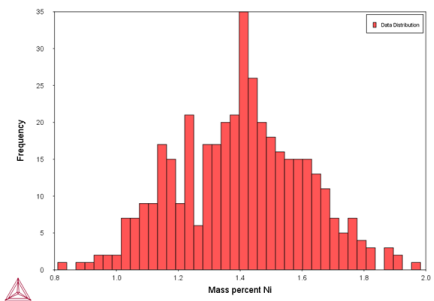
**Total samples = 200**



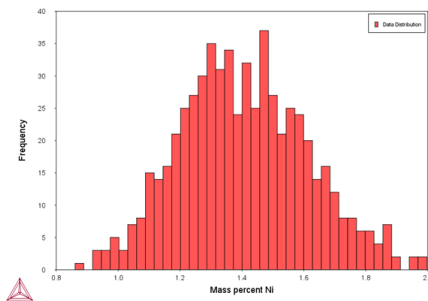
**Total samples = 300**



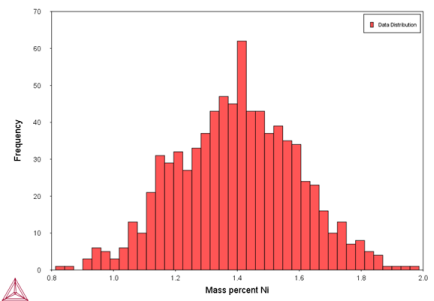
**Total samples = 400**



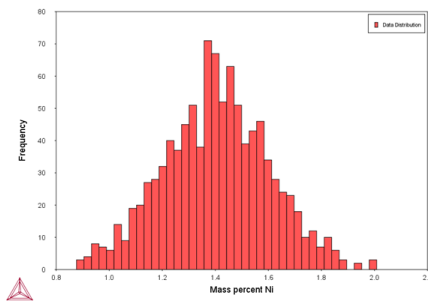
**Total samples = 600**



**Total samples = 800**



**Total samples = 1000**



## Normal Probability Plot

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

Property Model Calculator 1

Tie lines: 0 Legend option: On Legend style: None

**X Axis**

Axis variable: Mass percent Ni

Axis type: Linear

Limits: 500.0 to 3000.0 step 250.0 ☒ Automatic scaling

**Y Axis**

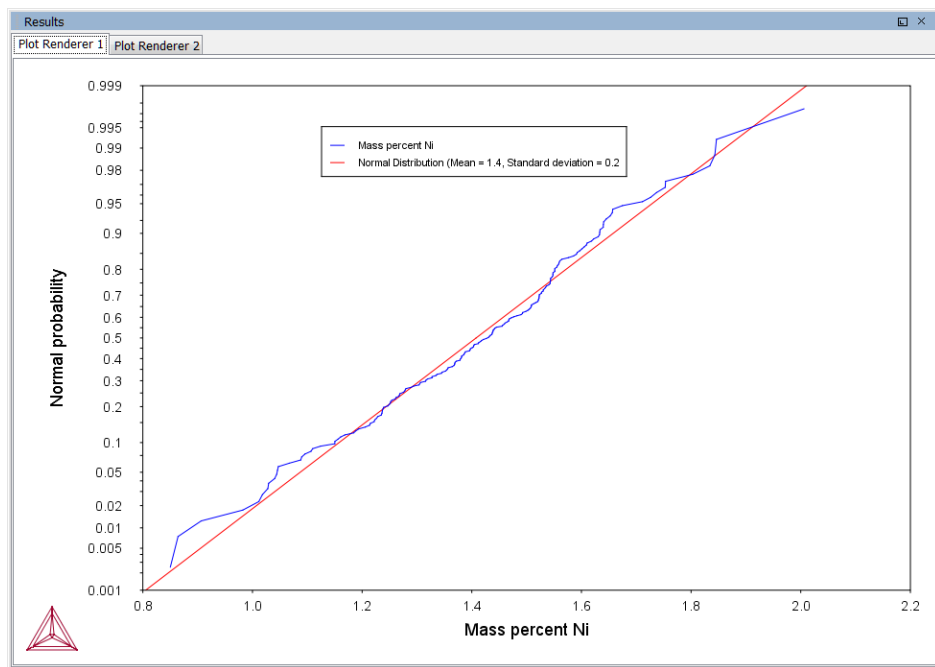
Axis variable: Normal probability

Axis type: Probability

Limits: 500.0 to 3000.0 step 250.0 ☒ Automatic scaling

☒

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



## Phase Transition Model

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

the phase transformation temperature, or composition, depending on the varied condition.



For an example of a phase transition model, see example 10 in [Graphical Mode Example Collection on page 9](#).

Define the:

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

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

## Driving Force Model

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

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

The calculation result is the driving force divided by  $RT$ .



For an example of a driving force model, see example 12 in [Graphical Mode Example Collection on page 9](#).

## Interfacial Energy Model

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

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

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



For an example of an interfacial energy model, see example 11 in [Graphical Mode Example Collection](#) on page 9.

### Estimation of Coherent Interfacial Energy

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

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

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

where  $\sigma_c$  is the coherent interfacial energy,  $n_s$  is the number of atoms per unit area at the interface,  $z_s$  is the number of cross bonds per atom at the interface,  $z_l$  is the coordination number of an atom within the bulk crystal lattice, and  $\Delta E_s$  is the energy of solution in a multicomponent system involving the two phases being considered. (Reference<sup>1</sup>).

## Coarsening Model

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

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

<sup>1</sup>Becker, R., Die Keimbildung bei der Ausscheidung in metallischen Mischkristallen, Ann. Phys. 424, 128–140 (1938).

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



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



For an example of a coarsening model, see example 11 in [Graphical Mode Example Collection on page 9](#).

## Particle Coarsening

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

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

Following Morral and Purdy, the rate constant of precipitating  $\beta$  phase in a multicomponent  $\alpha$  phase is

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

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

Using the u-fractions that is defined as

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

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

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

The interfacial energy  $\sigma$  is calculated using the extended Becker's model (that also is available as a separate Property Model Calculator model)

## References

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

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

## Equilibrium Model

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

## Equilibrium Calculator

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

- **Conditions:** Set the conditions for your calculation that define the stepping or mapping axis variables. This tab can be viewed in a simplified mode and in an advanced mode. See [Setting Equilibrium Calculator Conditions on the next page](#).
- **Functions:** Define your own quantities and functions, which you then can calculate and plot. See [Calculating and Plotting Functions on page 76](#).
- **Options:** Modify numerical settings that determine how equilibria are calculated, as well as how stepping and mapping calculations are performed.



The **Options** tab is where you can locally define specific Equilibrium Calculator settings. These are the same settings described in [Global Settings: Calculation \(Equilibrium Calculator\) on page 194](#).

See [Creating Activities and Successors on page 29](#) for a list of possible successors and predecessors for this activity. An Equilibrium Calculator that is the successor of another Equilibrium Calculator inherits all the Configuration window settings of the predecessor.



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

## Configuration Window

Configuration

**Equilibrium Calculator 1**

Conditions Functions Options

Composition unit: Mass percent Switch to advanced mode

**Condition Definitions**

Temperature: Kelvin 1000.0

Pressure: Pascal 100000.0

System size: Mole 1.0

Composition: Fe 99.98

Composition: C 0.01

Composition: Cr 0.01

**Calculation Type**

☐ Single equilibrium ☐ Property diagram ☐ Property grid ☒ Phase diagram

**Axis Definitions**

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

? 📄 < Add Predecessor Perform Create New Successor >

## Setting Equilibrium Calculator Conditions

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

The conditions to set depend on the type of calculation.



See [Graphical Mode Example Collection on page 9](#): Example 1 is a single-point equilibrium calculation; Example 2 is a stepping calculation; Example 5 is a mapping calculation.

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



## Setting Conditions for Simplified Mode

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

### The Conditions Tab

Conditions Functions Options

Composition unit Mass percent ▼

**Condition Definitions**

Temperature Celsius ▼ 1000.0

Pressure Pascal ▼ 100000.0

System size Mole ▼ 1.0

**Calculation Type**

☐ Single equilibrium ☐ Property diagram ☐ Property grid ☒ Phase diagram


**Axis Definitions**

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

### Conditions Tab, Simplified Mode Settings

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

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

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

### Calculating with a Fixed Phase (Advanced Mode)

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

### How to Calculate with a Fixed Phase



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

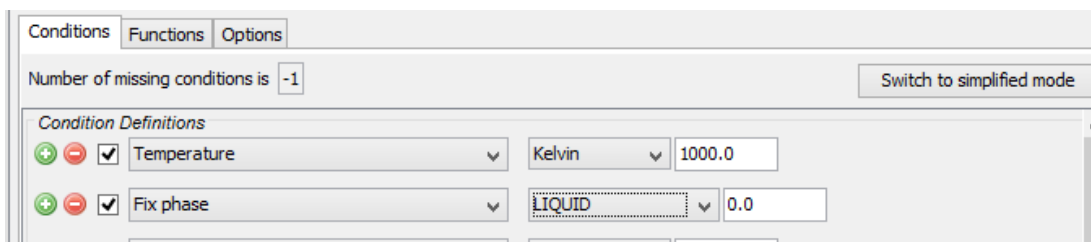
1. Right-click a node that can add an Equilibrium Calculator to your project. See [Creating Activities and Successors on page 29](#) for a list.
2. In the **Project** window, click the **Equilibrium Calculator** activity node.

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



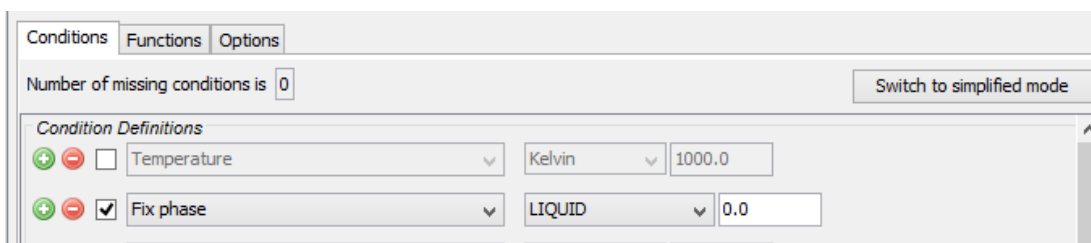
If the **Default calculation mode** is globally set to **Advanced** then by default the Configuration window is already in advanced mode. See [Changing Global Settings on page 187](#).

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



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

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



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


## Calculating and Plotting Functions

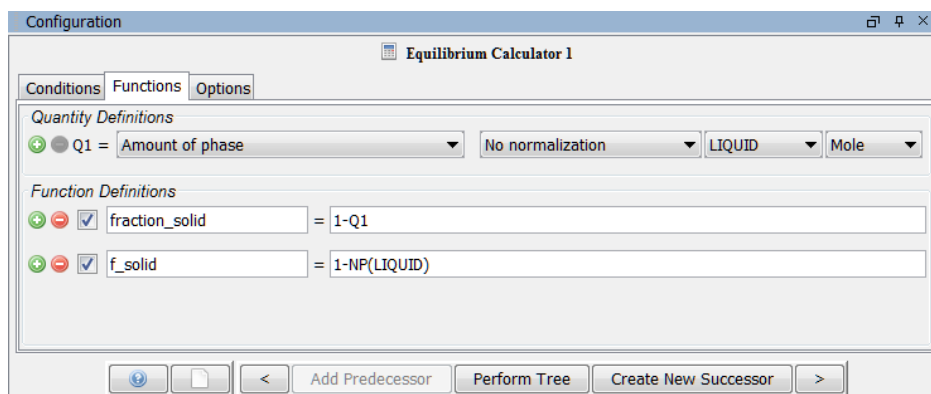
The **Functions** tab allows you to define your own functions that can be plotted in a Plot Renderer.




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

## How to Calculate and Plot Functions

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



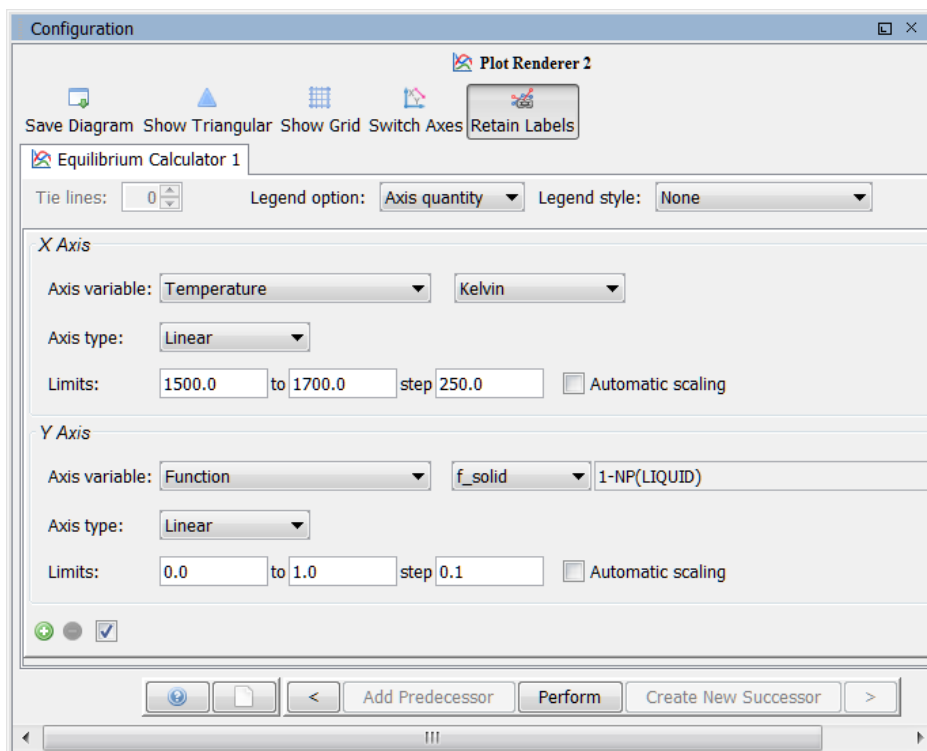
4. Under **Function Definitions**, click the add  button to add a new function. In the left field edit the default name of each function and enter the function itself in the right field after the equal sign. In this example, the quantity defined as Q1 is renamed to **fraction\_solid**, which gives as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



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

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

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



## Precipitation Calculator



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

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

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

### Configuration Window

#### Example

**Configuration** Precipitation Calculator 1

**Conditions** | Options

Composition unit: **Mass percent**

Composition Fe: 87.9  
Composition C: 0.1  
Composition Cr: 12.0

**Matrix Phase**  
Phase: BCC\_A2 Show details

**Precipitate Phase**  
Phase: CEMENTITE Show details  
Nucleation sites: Grain boundaries ☒ Calculate from matrix settings: 6.528500136483704E23 m<sup>-3</sup> Wetting angle (0-90): 90.0 °  
Interfacial energy: User-defined 0.174 J/m<sup>2</sup>

**Precipitate Phase**  
Phase: M23C6 Show details  
Nucleation sites: Grain boundaries ☒ Calculate from matrix settings: 6.528500136483704E23 m<sup>-3</sup> Wetting angle (0-90): 90.0 °  
Interfacial energy: User-defined 0.26 J/m<sup>2</sup>

**Precipitate Phase**  
Phase: M7C3 Show details  
Nucleation sites: Grain boundaries ☒ Calculate from matrix settings: 6.528500136483704E23 m<sup>-3</sup> Wetting angle (0-90): 90.0 °  
Interfacial energy: User-defined 0.3 J/m<sup>2</sup>

**Calculation Type**  
☐ Isothermal ☐ Non-isothermal ☒ TTT diagram

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

Add Predecessor Perform TTT Diagram Simulation Create New Successor

## Conditions Tab Settings

These are the settings on the Precipitation Calculator Conditions tab.

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

### Matrix Phase

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



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



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

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

### Precipitate Phase

**Phase:** Choose a phase from the list. The list is based on the settings for the System Definer.



The phases available to choose have both thermodynamic and kinetic data. If the list is empty, go to the System Definer to make sure that both types of databases are selected and defined. See "System Definer" in the *Thermo-Calc User Guide* or search the Online Help.

**Nucleation sites:** Choose one of the following from the list.

- **Bulk, Grain boundaries, Grain edges, Grain corners, or Dislocations.** Click to select the **Calculate from matrix settings** check box if you want to calculate the number density of sites.
- For Grain boundaries, Grain edges and Grain corners, enter the **Wetting angle** in addition to the matrix settings.
- To enter a specific value for the number of nucleation sites, deselect the check box.

**Interfacial energy:** Choose **Calculated** to use the estimated value and then enter a different **prefactor** value if you want to adjust the estimated value. You can also choose **User defined** to enter a value in J/m<sup>2</sup>.



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

- **Molar volume:** Choose the default to take the value from the **Database** or **User-defined** to enter another value. **Database** is available in the list when the molar volume for the phase is defined in the thermodynamic database.
- **Phase boundary mobility:** Enter a numerical value.
- **Phase energy addition:** Enter a numerical value.

- **Approximate driving force:** Select the check box to include this if simulations with several compositions sets of the same phase create problems.

## Calculation Type

### *Isothermal*

Use an **Isothermal** calculation type to do a precipitation simulation at constant temperature.

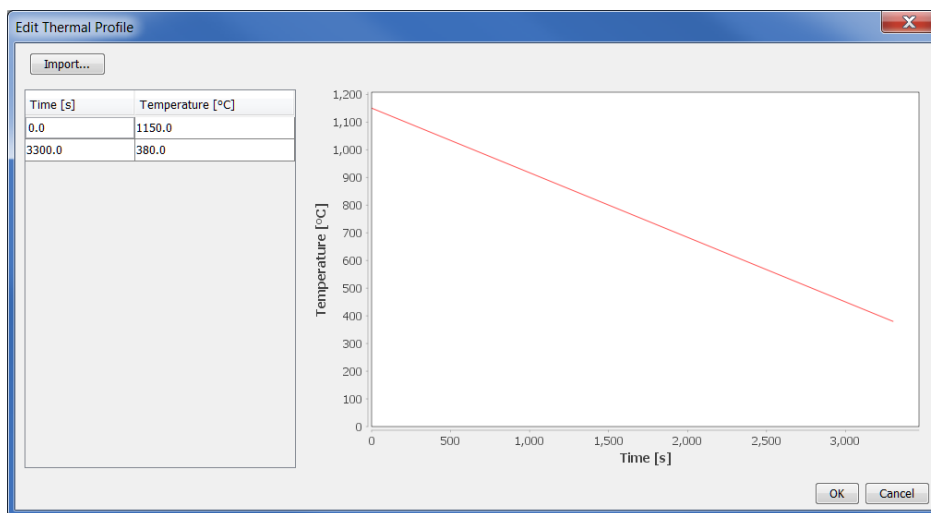
For the **Isothermal** calculation type, enter a **Temperature** and **Simulation time**.

### *Non-Isothermal*

For the **Non-isothermal** calculation type, select a **Temperature unit** and **Time unit** from the lists. Enter a value for the **Simulation time**.

Click **Thermal Profile** to define the heat treatment schedule. Here the **Temperature** and **Time** coordinates of thermal profile points are entered. A minimum of two points is required. You can also click **Import** to add your own thermal profile from an Excel spreadsheet.

## Edit Thermal Profile Window



### *TTT-Diagram*

Use a **TTT-diagram** calculation type to do a precipitation simulation of the time-temperature-transformation (TTT).

For the **TTT diagram** calculation type, enter **Min**, **Max**, and **Step** values for the **Temperature** and choose a **Unit** from the list.

**Max simulation time:** Enter a numerical value and choose a **Unit** from the list.

**Stop criterium:** Choose **Volume fraction of phase** or **% of equilibrium fraction** and then enter a numerical value in the field. For each temperature, the simulation stops when the stop criterium is



fulfilled or if the maximum simulation time is reached, whichever happens first.

## **Options Tab Settings**

These are the settings on the Precipitation Calculator Options tab.

---

## Settings

### Growth Rate Model

Choose from **Simplified** (the default) or **Advanced**.

### Numerical Parameters

Enter numerical values for the following as required.

- **Max time step fraction:** The maximum time step allowed for time integration as fraction of the simulation time.
- **No. of grid points over one order of magnitude in radius:** Default number of grid points for every order of magnitude in size space.
- **Max no. of grid points over one order of magnitude in radius:** The maximum allowed number of grid points in size space.
- **Min no. of grid points over one order of magnitude in radius:** The minimum allowed number of grid points in size space.
- **Max relative volume fraction of subcritical particles allowed to dissolve in one time step:** The portion of the volume fraction that can be ignored when determining the time step.
- **Max relative radius change:** The maximum value allowed for relative radius change in one time step.
- **Relative radius change for avoiding class collision:** Set a limit on the time step.
- **Max overall volume change:** This defines the maximum absolute (not ratio) change of the volume fraction allowed during one time step.
- **Max relative change of nucleation rate in logarithmic scale:** This parameter ensures accuracy for the evolution of effective nucleation rate.
- **Max relative change of critical radius:** Used to place a constraint on how fast the critical radius can vary, and thus put a limit on time step
- **Min radius for a nucleus to be considered as a particle:** The cut-off lower limit of precipitate radius.
- **Max time step during heating stages:** The upper limit of the time step that has been enforced in the heating stages.

## Plot Renderer

The Plot Renderer displays results from the various calculator activities .

The available Plot Renderer functionality varies by calculation type. For example:

- If you choose a *Property grid* (Equilibrium Calculator) or *Grid* (Property Model Calculator) calculation type, select a **Plot type** and whether to **Interpolate** the data or not.
- For a Property Model Calculator *Uncertainty* calculation type, you choose an **Axis type**: **Frequency**, **Histogram** or **Normal probability**. For other calculators (e.g. Equilibrium, Binary, and Scheil) there are different axis types available such as **Linear**, **Logarithmic**, **Logarithmic 10**, and **Inverse**.

The Plot Renderer is used to set the plotting axis variables for a property diagram and phase diagram.

If you are plotting a Property grid (Equilibrium Calculator) or Grid (Property Model Calculator) then the X- and Y-axes always represent the quantities that define the stepping axes, but you need to set a variable for the Z-axis (the axis perpendicular to the plane defined by the X- and Y-axes).



Also see [Creating Activities and Successors on page 29](#) for a list of possible successors and predecessors for this activity.

The configurations that can be set in the Configuration window for a Plot Renderer vary depending on the kind of predecessor it is created from.

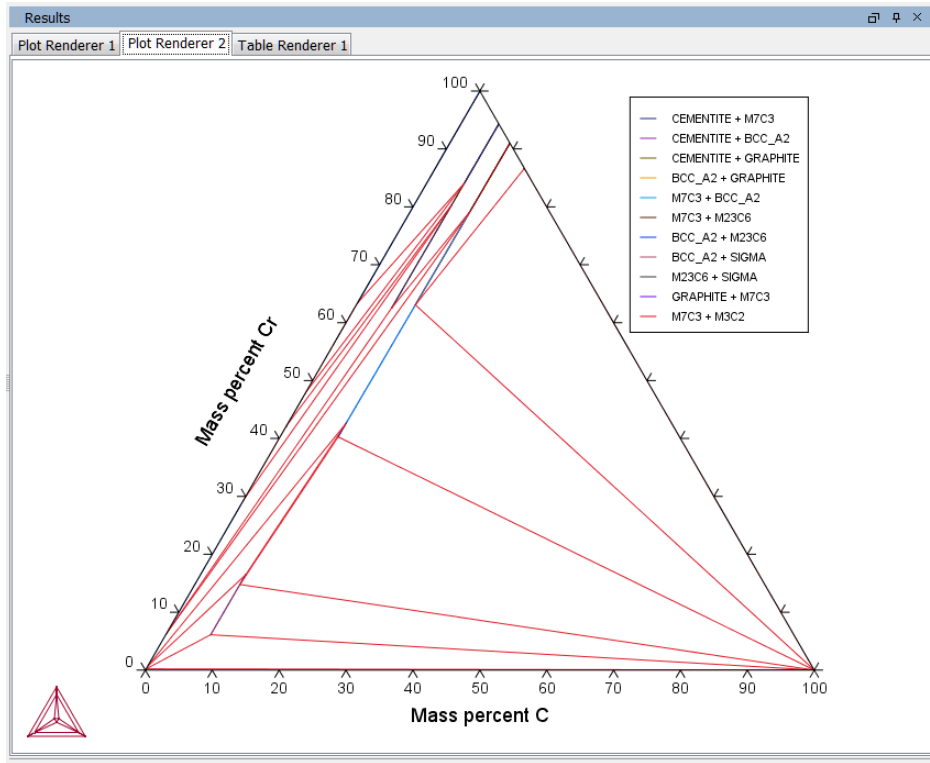
### Plot Several Calculations in One Diagram

A Plot Renderer can have several predecessors (if you want to plot several calculations in the same diagram), in which case there are several tabs in the Configuration window, one for each predecessor.

Several Plot Renderer activities (as well as Table Renderer activities) can be shown in the Results window as different tabs. The figure is from Graphical Mode example 4.



Also see [Plotting Several Calculations in One Diagram on page 96](#) for details.



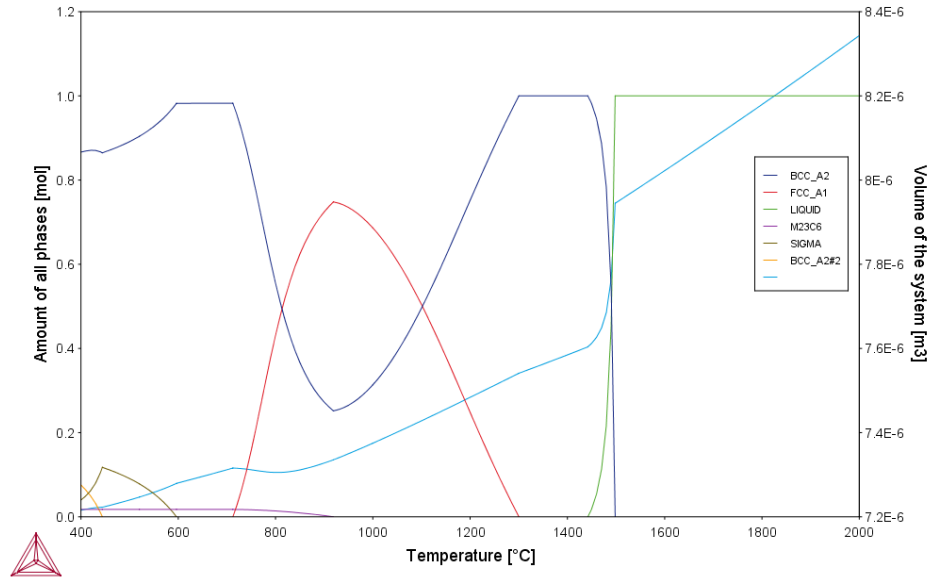
## Add Axes to Diagrams

You can add additional X- and/or Y-axes to a plot to compare two or more variables at the same time as in the figure.



Also see [Adding Axes to a Diagram on page 97](#) for details.

*Two variables plotted on the Y-axis.*



### Merge Results in One Diagram

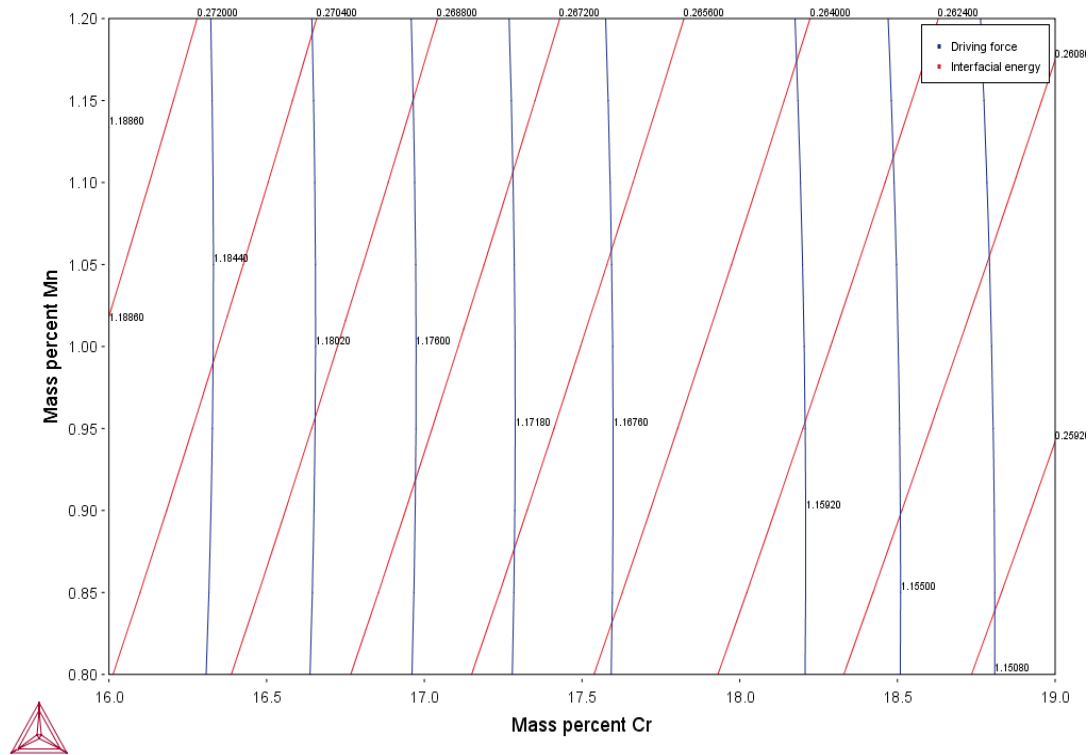
You can merge (or overlay) calculated results for several variables into one diagram. This is similar to adding an axis, but instead of displaying different variables along the X- and/or Y-axes, the same X and Y variables are used to compare the third variable (defined in the Plot Renderer as the Z-axis).

As in the figure (from example 12 in Graphical Mode Examples), the driving force and interfacial energy results are combined into one diagram. The X and Y axis is the same for both (Mass percent Cr/Mass percent Mn).



Also see [Merging Plots into One Diagram](#) on page 99 for details of how to combine diagrams.

*A contour plot showing both the driving force and interfacial energy calculation results comparing Mass percent Cr to Mass percent Mn.*



## Configuration Window

The Configuration window has different options available based on its predecessor. The following is an example of the Configuration window for a Plot Renderer that is the successor to an Equilibrium Calculator. The options along the top are available for most of the calculation types (e.g. phase diagrams, property diagrams, min/max, uncertainty and so forth). For an Equilibrium Property Grid calculation type and a Property Model Calculator Grid calculation you can choose a **Plot type**.

Configuration

Plot Renderer 1

Save Diagram Show Triangular Show Grid Switch Axes Retain Labels

Property Model Calculator: Coarsening

Tie lines: 0 Plot type: Heat map Interpolate: Never

**X Axis**

Axis variable: Mass percent Cr

Axis type: Linear

Limits: 500.0 to 3000.0 step 250.0 ☒ Automatic scaling

**Y Axis**

Axis variable: Mass percent C

Axis type: Linear

Limits: 500.0 to 3000.0 step 250.0 ☒ Automatic scaling

**Z Axis**

Axis variable: Coarsening rate coefficient

Axis type: Linear






Limits: 500.0 to 3000.0 step 250.0 ☒ Automatic scaling




+

Perform




Add Predecessor Create New Successor

## Configuration Settings

Setting/Button	Description
Save Diagram  Save Diagram	Save the plot diagram.
Show Triangular  Show Triangular	Display the diagram in triangular form, with the X-axis along the base and the Y-axis along the left side. Such a diagram is often useful if you want to plot the fractions of two components in a ternary diagram.
Show Grid  Show Grid	Overlay a grid on the diagram.
Switch Axes  Switch Axes	Show the plotting X axis variable on the diagram's Y-axis, and the Y axis variable on the diagram's X-axis.
Retain Labels  Retain Labels	Toggle the default to keep labels displaying on the plot. By default labels are retained.

Setting/Button	Description
Tie lines	<p>Select how many tie lines to be plotted in the diagram. Every nth number of tie line is plotted, where n is the number set here. Consequently, the higher the number, the fewer the number of plotted tie lines in the diagram.</p> <p> This setting is not available if the Plot Renderer is a successor to a Precipitation Calculator, Scheil Calculator or to an Equilibrium Calculator where only one axis is defined and varied (that is, an Equilibrium Calculator that has performed a stepping calculation).</p>
Legend option	Select whether the diagram's legend displays the Stable phases, the Axis quantity, or choose Off for no legend.
Legend style	<p>You can select a Legend style for the <b>Stable phases</b> or <b>Axis quantity</b> selected for <b>Legend option</b>. Choose <b>None</b>, <b>All</b>, <b>Constitution description</b>, or <b>Ordering description</b>.</p> <p> Also see <a href="#">About Legend Styles on page 91</a>.</p>
Plot type (property grid or grid)	<p> This menu is available if the Plot Renderer is a successor to either an Equilibrium Calculator that is set up to calculate a <i>Property grid</i> or a Property Model Calculator that is calculating a <i>Grid</i>.</p> <p>On a <b>Heat map</b> diagram, each equilibrium calculation in the grid is represented by a colour-coded pixel, where dark red represents the highest Z-axis variable value and dark blue represents the lowest Z-axis variable value.</p> <p>On a <b>Contour</b> diagram, Z-axis variable values are traced with curves in different colours (in the same way that height values are traced with curves on a topographical map).</p> <p>From the <b>Interpolate</b> list, choose to interpolate data <b>Never</b> (the default), <b>Once</b>, <b>Twice</b> or <b>3 times</b>. This means points are put in between calculated points in the grid and interpolated instead of calculated in the calculation engine.</p>
Interpolate (property grid or grid)	Choose how many points of data to interpolate on a grid or property grid to improve curve smoothness – <b>Never</b> , <b>20x20</b> , <b>50x50</b> , or <b>100x100</b> . Try different settings for your own set of data.



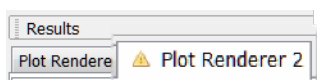
Setting/Button	Description
Axis variable	<p>Set the state variable you want plotted along the X-axis and the Y-axis.</p> <p> If the stepping/mapping variables are changed in the Equilibrium Calculator that precedes the Plot Renderer, then the variables to be plotted along the diagram's X- and Y-axis are automatically updated to the appropriate quantities.</p> <p>For a Precipitation Calculator:</p> <ul style="list-style-type: none"> <li>• Select the <b>Separate multimodal PSD</b> check box to enter settings for <b>Points</b>, <b>Excess kurtosis</b>, <b>Valley depth ratio</b> and <b>Minimum peak</b>.</li> </ul>
Axis type	Select what type of scale to use on the axis. Choose between <b>Linear</b> , <b>Logarithmic</b> , <b>Logarithmic 10</b> or <b>Inverse</b> .
Limits	<p>Specify the range along the axis that is shown in the plot by setting the minimum and maximum values of the axis variable. You can also determine the step size between the tick marks along each axis.</p> <p>Alternatively, select Automatic scaling.</p>
Unit ( <i>Time X Axis</i> )	For a Precipitation Calculator choose a <b>Unit</b> - <b>Seconds</b> , <b>Hours</b> , or <b>Days</b> .
Add an axis  and Remove this axis  buttons.	Use these buttons to add additional X- and/or Y-axes to a plot or to merge plots (to overlay one plot with another in the same diagram). When merging plots, you define this variable as the Z-axis. See Adding Axes to a Diagram and Merging Plots into One Diagram for details.

### Plot Status Marker

If you have plotted a diagram and then modify something in the tree that the Plot Renderer is associated with, then a notification sign—an exclamation mark enclosed in a yellow triangle—is shown in the Plot Renderer's tab.



Also see [Node Status Markers](#) on page 40.



## About Legend Styles

There are a variety of legend styles you can use to display detail about the phases.

The same legend styles are available for both Graphical Mode and Console Mode plots. For Console Mode, use the command `CHANGE_LEGEND` in the *Thermo-Calc Console Mode Command Reference Guide*.

In Graphical Mode the label styles are defined when using the [Plot Renderer on page 83](#). You can select a **Legend style** for the **Stable phases** or **Axis quantity** selected for **Legend option**.

When there is a legend in the diagram you can append constitution and/or ordering descriptions to the phase name.

If constituent description is included in the legend, then for each equilibria along a line in the diagram, the largest constituent fractions are summed until they are equal or greater than 0.6. This is done separately for each sublattice. If the equilibria along the line gets different sets of constituents these are all appended to the list for that sublattice.

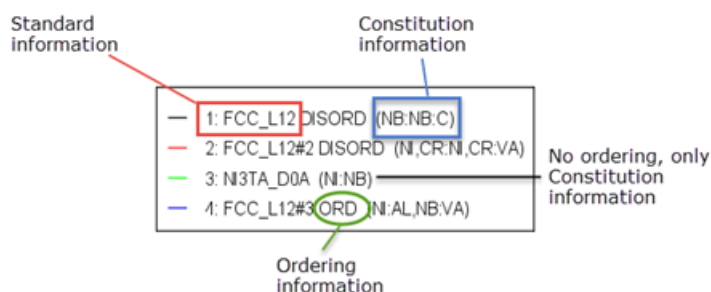
The ordering description is only printed for partitioned phases (phases that have a disordered contribution) that begins with at least two identical sublattices (sublattices where the set of constituents are identical). `DISORD` (disordered) is shown if site fractions are identical between identical constituents on all identical sub lattices (with an error margin) otherwise `ORD` (ordered) is shown in the legend.

If ordering between equilibria in a line are different, then `ORD + DISORD` is shown in the legend.

### Legend Examples

To show the differences between labels, the following uses the same example file that creates Figure 6 in [TCNi8 database extended information](#) document (found on the Thermo-Calc website).

When **All** is selected for this specific example the label includes the following:



Specifically:

- There are two disordered FCC phases (matrix and carbide), one ordered FCC (gamma prime), plus a phase NI3TA\_D0A (called Delta in Ni-alloys).
- ORDERING shows the different FCC phases.

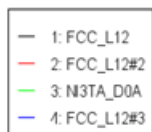
- CONSTITUTION shows that FCC\_L12#1 is NbC, FCC\_L12#2 is matrix with Ni and Cr as major constituent, FCC\_L12#3 is Ni<sub>3</sub>Al with Nb addition and NI3TA\_D0A is Nb-rich (eg. Ni<sub>3</sub>Nb).

### Label Style Choice Examples

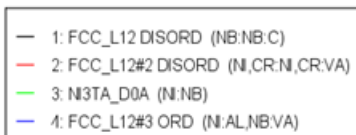
These examples are for each label style choice - None, All, Constitution or Ordering

The instructions are for when you are setting the options using the Plot Renderer. In Console Mode, you choose the options (ALL, NONE, CONSTITUTION, or ORDERING) after the command CHANGE\_LEGEND.

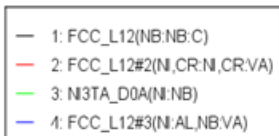
When **None** is selected the legend includes the standard information about the phases.



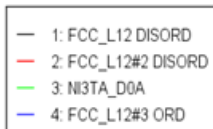
When you select **All** the **Constitution description** and the **Ordering description** (when there is ordering) are included.



When you select **Constitution description**, this is added to the standard description.



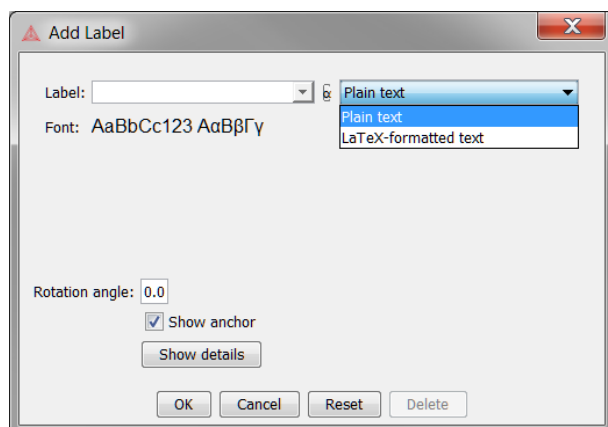
When you select **Ordering description** and when there is ordering, this is added to the standard description.



### Adding and Editing Plot Labels

To add a label text at a certain point in a plot, right click the point, and select **Add Label**. For phase diagrams, the program suggests a label that you can keep or edit. The suggested label specifies the names of the stable phases at the coordinate where you clicked. For all other plot types, you enter your own text, which can either be Plain text or LaTeX formatted text.

### Add Label Window



### Label Formatting

You can enter the label as **Plain text** or in **LaTeX-formatted text**. For **LaTeX-formatted text** enter or edit the text as required. For example, underscores ( `_` ) are added before the numbers to make subscripts in the label.



For a list of supported LaTeX commands, see:

<http://www2.ph.ed.ac.uk/snuggletex/documentation/math-mode.html>.

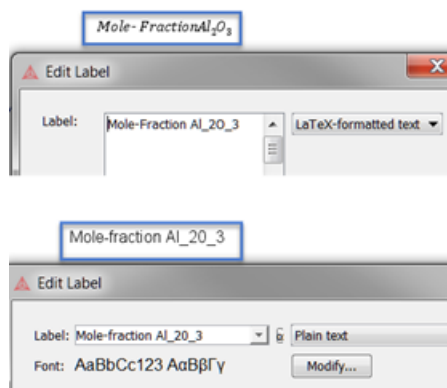


By default when using LaTeX, you are in math mode and Thermo-Calc automatically interprets the entered text as math. The above link uses the dollar sign (\$) in all the examples but this is NOT required. For example, if you enter  $E=mc^2$  this is displayed including the \$ instead of the equation.

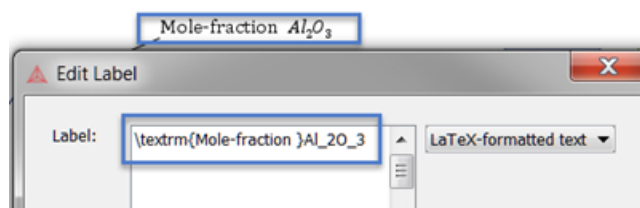
### Entering a Mixture of Plain Text and Equations

When you enter text using LaTeX formatted text it displays by default on the plot in italics and treats the text as an equation.

As in the following example, the top label does not display correctly because the label is a mixture of text (Mole-Fraction) and an equation ( $\text{Al}_2\text{O}_3$ ). In the bottom image, when the same information is added as Plain text to the plot it now does not include the subscripts.



To add a mixture of plain text and equation text, you can exit math mode using the string `\textrm` followed by the text to display enclosed in curly brackets. For example `\textrm{Mole-fraction }Al_2O_3` results in the label as shown:



In this example, you need to add a space at the end of fraction in order to separate the text from the equation part of the label.



When working in Console Mode, you can also use the above windows on the Console Results window to add and edit labels. In addition, you can use the `ADD_LABEL_TEXT` command described in the *Thermo-Calc Console Mode Command Reference*.

### Rotation Angle and Show Anchor

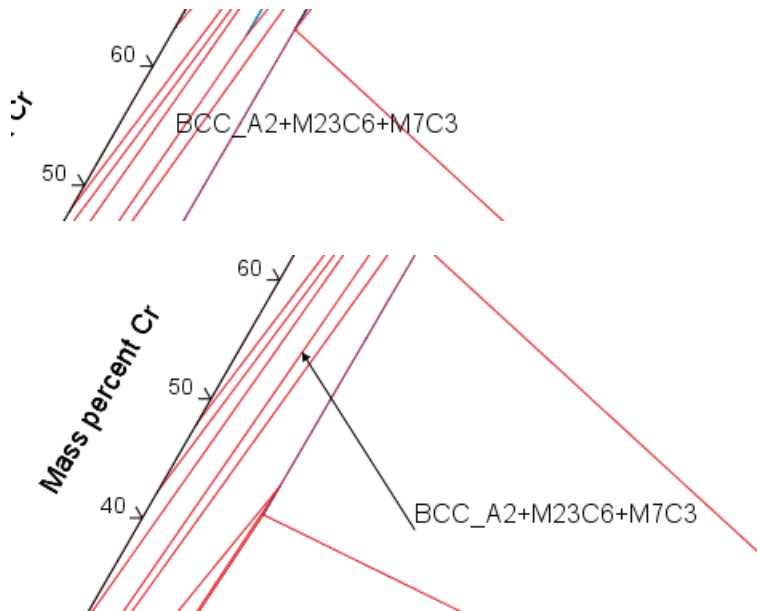
By default the **Show anchor** check box is selected, which includes an arrow from the label point to the coordinates.

If you do not want the label oriented horizontally in the Plot Renderer tab, then specify the number of degrees of rotation in the **Rotation angle** field.

Click **OK** to add the label to the plot. You can also move a label by clicking and dragging it. The default anchor arrow is added to indicate the point that belongs to the label.

### Moving Labels in a Plot

Drag and drop labels anywhere on the plot. The anchor arrow points to the point of origin.

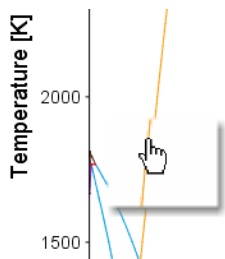


## Changing the Plot Properties

For global changes to the default settings plots see [Global Settings: Graphical and Console Mode-Plotting on page 200](#). The settings are the same but applied to all new plots.

To make local changes to the appearance of a specific plot, in the **Results** window right-click a plot and select **Properties**. You can also edit some properties for individual plot lines (the color, the line width and type, and whether data points are included).

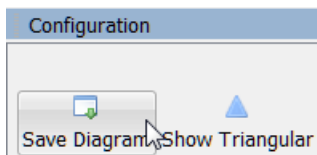
In the **Results** window, hover the mouse over a plot line. When it is over a line that can be clicked the crosshair cursor turns into a pointing finger.



To prevent unintended edits, hold down <Ctrl> while moving the cursor around the plot to only display it as a crosshair.

## Saving Plots

1. To save a diagram, at the top of the **Configuration** window click **Save Diagram**.



Or right-click the diagram in the **Results** window and select **Save As**.

2. In the **Save** window, navigate to where you want to save the plot, enter a **File name**, and choose the **File type** to save it in. Click **Save**.

## Plotting Several Calculations in One Diagram

You can plot several calculations in the same diagram by adding extra predecessors to the Plot Renderer activity.

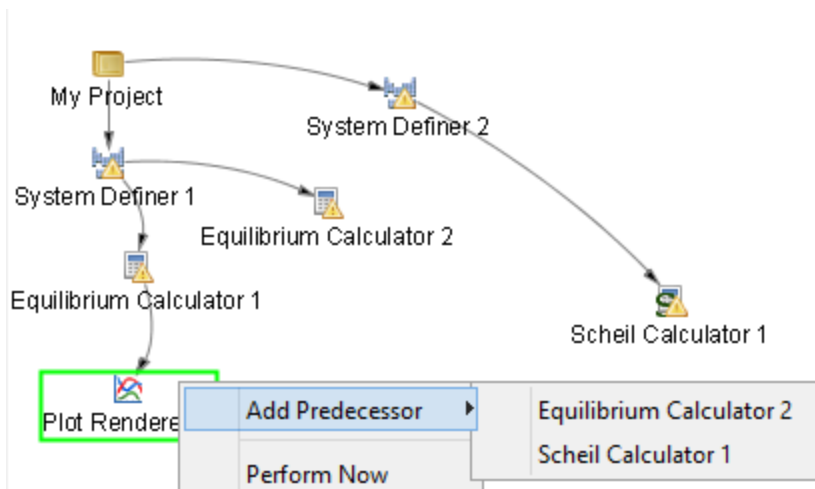


For an example of a project in which several calculations are plotted in one diagram, see example 5 in [Graphical Mode Example Collection on page 9](#).

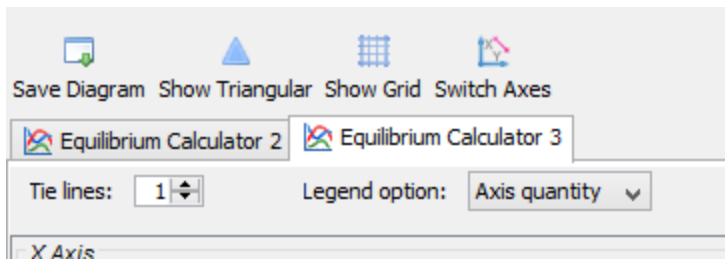
To plot several calculations in one diagram, you must have, in addition to the Plot Renderer's original predecessor, at least one available Plot Renderer predecessor in your project. The extra predecessor can be any of these: Equilibrium Calculator, Binary Calculator, Ternary Calculator, Scheil Calculator or Experimental File Reader.

### How to Plot Several Calculations in One Diagram

1. In the Project window click the **Plot Renderer** node.
2. In the **Configuration** window click **Add Predecessor**. Or right-click the **Plot Renderer** and choose **Add Predecessor**.

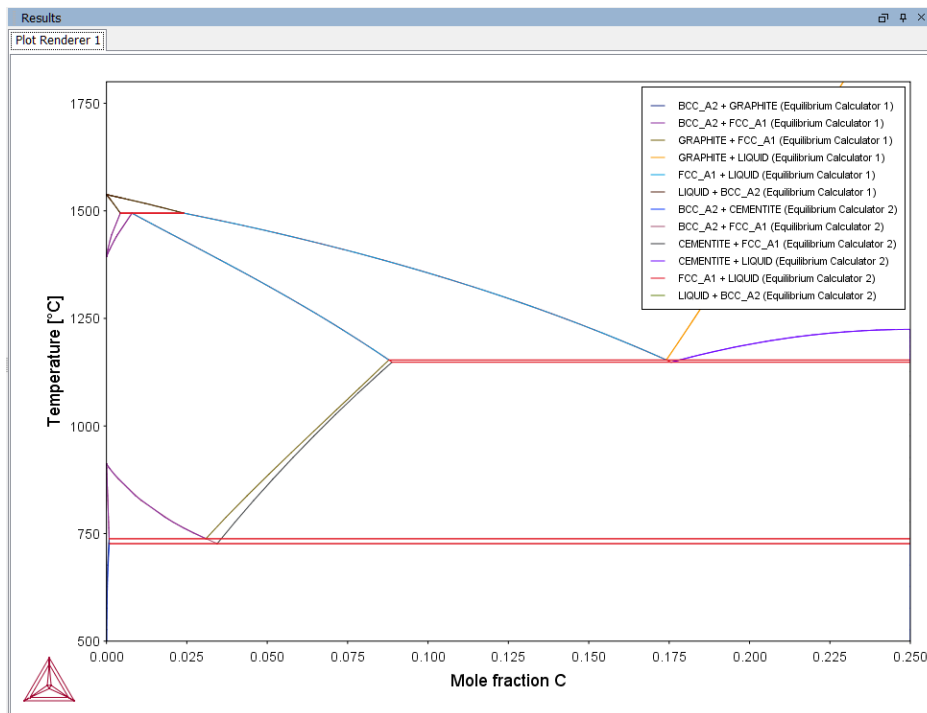


3. Select a predecessor. When added, the extra predecessor is linked to the Plot Renderer. On the Plot Renderer's Configuration window, the predecessors are shown as two tabs:



4. Configure how you want each calculation plotted on the tabs in the **Configuration** window, then click to **Perform** the Plot Renderer activity.


The calculations are plotted in the same diagram in a tab in the **Results** window. If any of the axis variables of the plots differ, then the label and scale of all calculations are shown parallel to each other. The following screen shot shows a diagram in which two calculations with different plotting axes variables have been plotted.



## Adding Axes to a Diagram

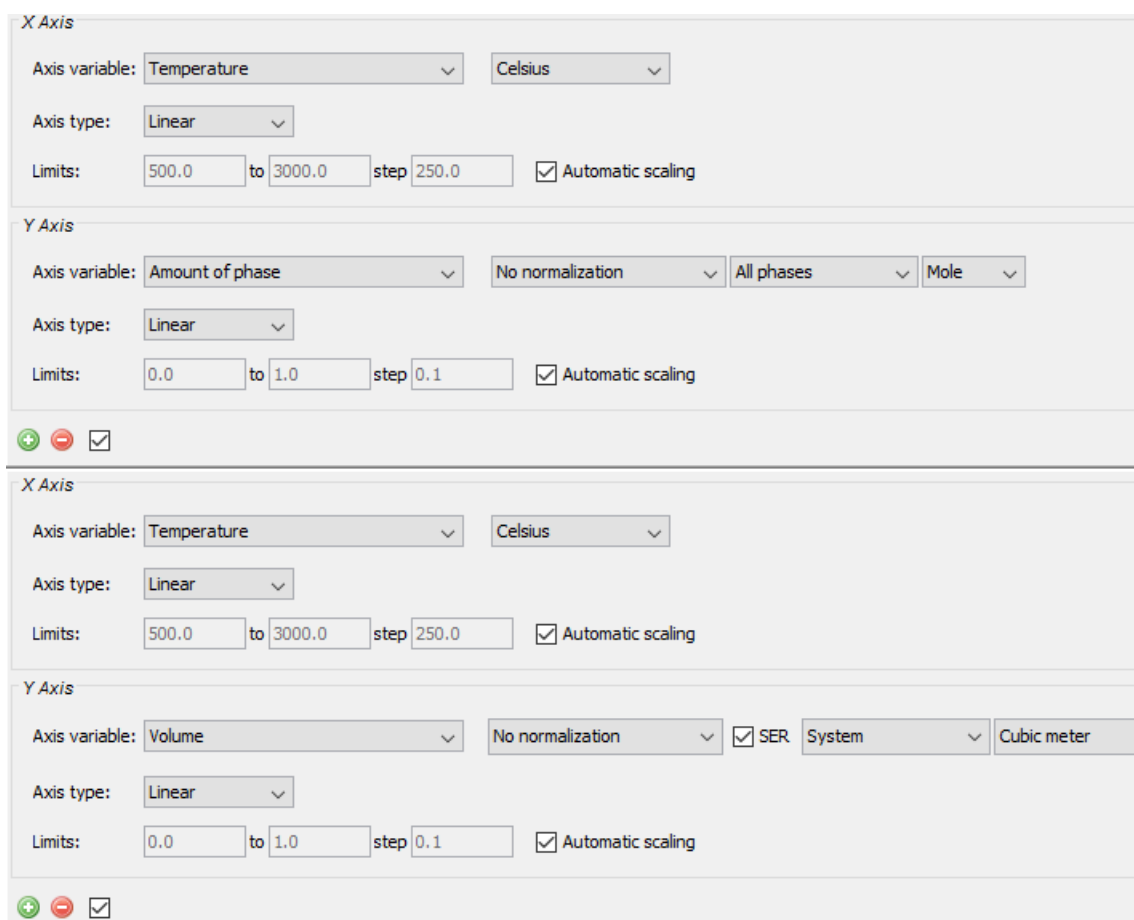
You can add additional X- and/or Y-axes to a plot to compare two or more variables at the same time.



1. In the **Project** window right-click the calculator node (e.g. an Equilibrium Calculator) and add a **Plot Renderer** node from the **Create New Successor** menu.
2. Click the **Plot Renderer** node.
3. In the **Configuration** window, define the plot. Available settings are based on the calculation type.
4. Click the **Add an axis**  button. A new settings section is added underneath.
5. From the *X Axis* and/or *Y Axis* sections define another **Axis variable** and choose an **Axis type**.
6. Click **Perform** to plot both variables on the selected axis, in this example, the Y-axis.

### Axis Example

In this example **Amount of phase** and **Volume** are selected as the Y-axis variables and **Temperature** as the X-axis variable.



The screenshot shows the 'Configuration' window with two axis settings sections. Each section has an 'X Axis' and a 'Y Axis' configuration area.

**Top Section:**

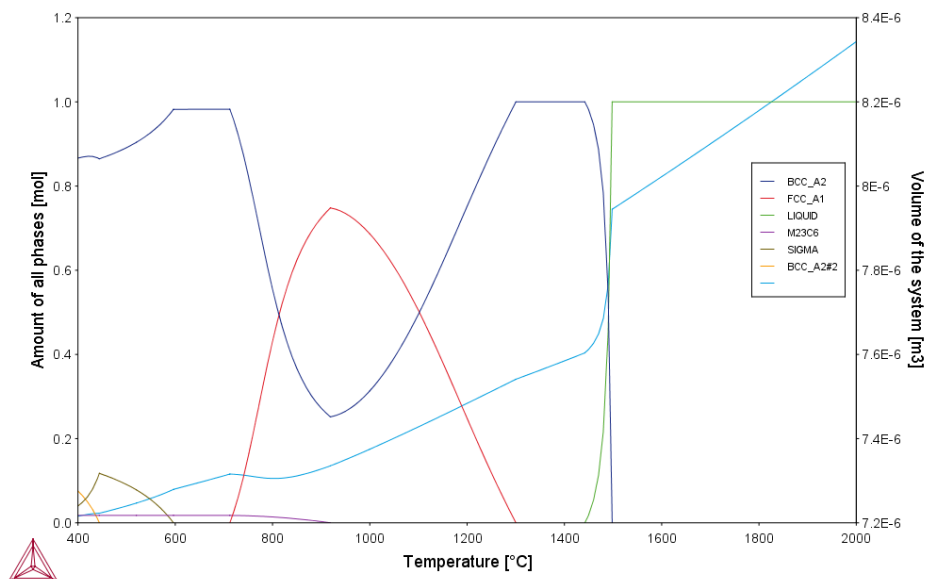
- X Axis:**
  - Axis variable: Temperature
  - Axis type: Linear
  - Limits: 500.0 to 3000.0 step 250.0
  - ☒ Automatic scaling
- Y Axis:**
  - Axis variable: Amount of phase
  - Axis type: Linear
  - Limits: 0.0 to 1.0 step 0.1
  - ☒ Automatic scaling

**Bottom Section:**

- X Axis:**
  - Axis variable: Temperature
  - Axis type: Linear
  - Limits: 500.0 to 3000.0 step 250.0
  - ☒ Automatic scaling
- Y Axis:**
  - Axis variable: Volume
  - Axis type: Linear
  - Limits: 0.0 to 1.0 step 0.1
  - ☒ Automatic scaling

Between the two sections, there are three buttons: a green plus icon, a red minus icon, and a checkmark icon.

### Plot Example



## Merging Plots into One Diagram

You can merge (or overlay) calculated results for several variables into one diagram. The same X and Y variables are used to compare the third variable (defined in the Plot Renderer as the Z-axis).



You cannot overlay heat map or frequency plots.

The following uses example 12 in Graphical Mode Examples to describe the steps to overlay two plots: the driving force and interfacial energy results are combined into one diagram. The X and Y axis is the same for both (Mass percent Cr/Mass percent Mn).

1. In the **Project** window right-click the calculator node (e.g. Property Model Calculator) and add a **Plot Renderer** node from the **Create New Successor** menu.
2. Click the **Plot Renderer** node.
3. In the **Configuration** window, define the plot. Available settings are based on the calculation type.

### Example

In this example the Property Model Calculator is set to a *Grid* calculation type.

Choose **On** for the **Legend** option and **Contour** as the **Plot type**.

**X Axis**

Axis variable: Mass percent Mn

Axis type: Linear

Limits: 0.0 to 100.0 step 10.0 ☒ Automatic scaling

**Y Axis**

Axis variable: Temperature Celsius

Axis type: Linear

Limits: 500.0 to 3000.0 step 250.0 ☒ Automatic scaling

**Z Axis**

Axis variable: Driving force

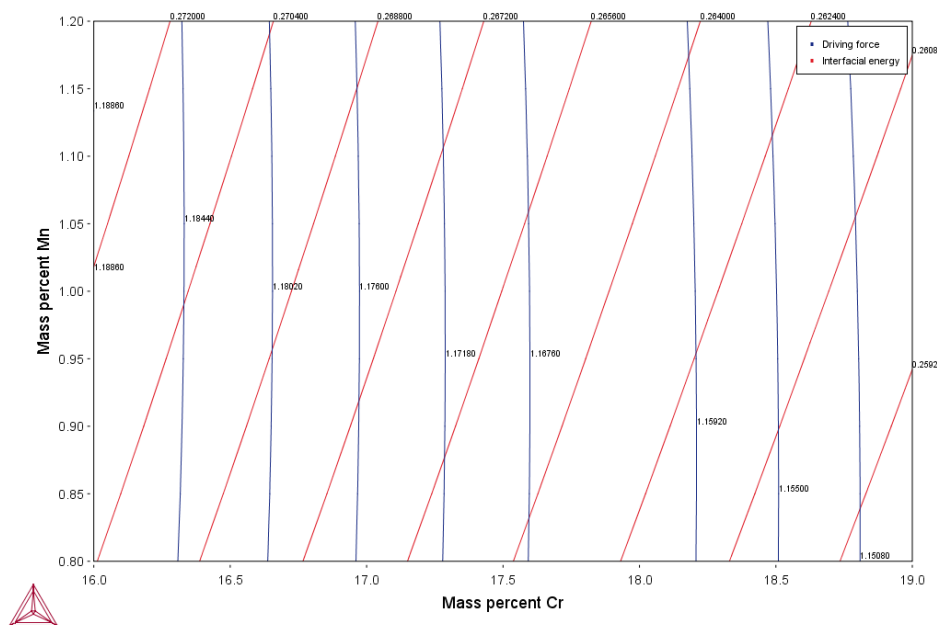
Axis type: Interfacial energy

Limits: 0.0 to 1.0 step 0.1 ☒ Automatic scaling

4. Click the **Add an axis** button. A new axes settings section is added underneath.
5. From the Z Axis section choose the **Axis variable**. In this example, **Interfacial energy**.
6. Click **Perform** to plot both on the same diagram.

### Plot Example

In this case, a contour plot showing both the driving force and interfacial energy calculation results comparing Mass percent Cr to Mass percent Mn.



## Table Renderer

A Table Renderer visualizes calculation results in a table. Several Table Renderer activities (as well as Plot Renderer activities) can be shown in the Results window as different tabs.

You can only successfully tabulate the results of a single-equilibrium calculation or a stepping operation. The tabulated data from an equilibrium calculation is different from the tabulated data from a stepping calculation.



Also see [Creating Activities and Successors on page 29](#) for a list of possible successors and predecessors for this activity.

## Tabulated Results from an Equilibrium Calculation

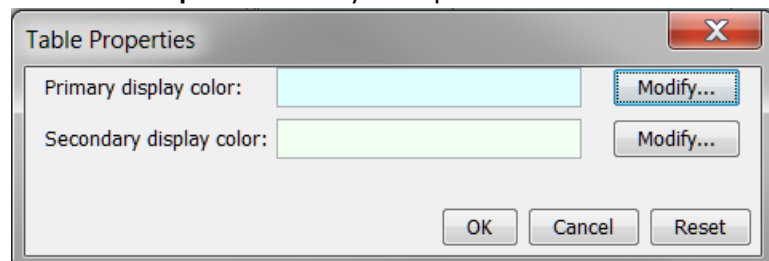
The following tab shows the result of an equilibrium calculation (from example 1 in [Graphical Mode Example Collection](#) on page 9).

Table Renderer 1				
<b>System</b>				
Moles	1.00000			
Mass	55.64392	[g]		
Temperature	1000.00000	[K]		
Total Gibbs Energy	-42140.55264	[J]		
Enthalpy	24707.16903	[J]		
Volume	7.29746E-6	[m3]		
<i>Component</i>	<i>Mole Fraction</i>	<i>Mass Fraction</i>	<i>Activity</i>	<i>Potential</i>
Fe	0.99537	0.99900	0.00619	-42277.77189
C	0.00463	0.00100	0.21818	-12658.35450
<b>Stable Phases</b>				
	<i>Moles</i>	<i>Mass</i>	<i>Volume Fraction</i>	
<b>BCC_A2#1</b>	0.99609	55.59691	0.99711	Composition and constitution ▼
<b>Composition</b>				
<i>Component</i>	<i>Mole Fraction</i>	<i>Mass Fraction</i>		
Fe	0.99928	0.99984		
C	0.00072	0.00016		
<b>Constitution</b>				
	<i>(Fe)<sub>1</sub>(C,VA)<sub>3</sub></i>			
	<i>Constituent</i>	<i>Site Fraction</i>		
<i>Sublattice 1:</i>				
	Fe	1.00000		
<i>Sublattice 2:</i>				
	VA	0.99976		
	C	0.00024		

For each stable phase listed, from the **Composition and constitution** menu you can select the information to view. In this example, the maximum amount of information is shown and includes details about both composition and constitution for **BCC\_A2#1**.

## Setting Background Colours

To change the background colours of the table, in the **Results** window right-click a Table Renderer tab, and select **Properties**. Modify as required.

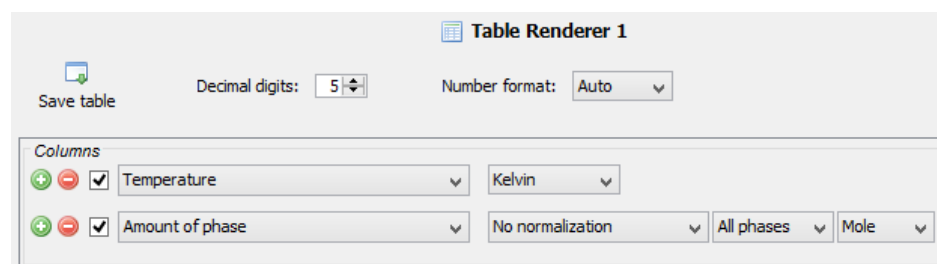


## Tabulated Results from a Stepping Operation

The **Table Render 1** tab in the example shows the results of a stepping calculation (from example 2 in *Graphical Mode Example Collection* on page 9).

Results				
Plot Renderer 1 Table Renderer 1				
Temperature [K]	Amount of BCC_A2 [mol]	Amount of LIQUID [mol]	Amount of FCC_A1 [mol]	Amount of GRAPHITE [mol]
1000.00000	0.99609			0.00391
1010.00000	0.99618			0.00382
1011.17278	0.99620			0.00380
1011.17278	0.99620		0.00000E0	0.00380
1011.17278	0.87364		0.12636	0.00000E0
1011.17278	0.87364		0.12636	
1020.00000	0.86046		0.13954	
1030.00000	0.84331		0.15669	
1040.00000	0.82356		0.17644	
1050.00000	0.80082		0.19918	
1060.00000	0.77395		0.22605	
1070.00000	0.74180		0.25820	

## Configuration Window Settings



## Defining the Table Columns

In the **Configuration** window for the Table Renderer 1 node, set the level of detail for the Columns:

### Setting Number Format and Number of Decimal Digits

The table results can be presented in ordinary decimal number format or with normalized scientific

notion. The **Number format** menu defaults to **Auto** to use the most appropriate format based on the tabulated data. Or choose **Scientific** or **Decimal** to increase or decrease the number of **Decimal digits** used in the table.

### Saving Tabulated Data

To save all the data in a table as a plain text file, in the **Configuration** window click **Save table** or in the **Results** window right-click in the table and select **Save As**.

To copy the data from a single cell of a table to the clipboard, right-click the cell and select **Copy**. To copy the whole table to the clipboard, select **Copy all**.



The data saved is what is shown in the **Table Renderer** tab. If data is calculated but not displayed it is not saved.

## Experimental File Reader

The Experimental File Reader activity can only be created from the top My Project node. This activity allows you to read an experimental data file (\*.EXP). This type of file has information specifying a plotted diagram, written in the DATAPLOT graphical language.



Also see [Creating Activities and Successors on page 29](#) and the *DATPLOT User Guide* included with this documentation set.

### How to Plot an Experimental Data File

1. Right-click **My Project** and from the **Create New Activity** submenu choose **Experimental File Reader**.
2. In the **Configuration** window in the **EXP file** field, enter the name of the EXP-file to plot.
3. Click **Create New Successor** and select **Plot Renderer**. Or right-click the **Experimental File Reader** node and from the **Create New Successor** submenu choose **Plot Renderer**.
4. In the **Configuration** window click **Perform** or right-click the **Plot Renderer** node and select **Perform**.

## Binary Calculator

A Binary Calculator can be used for some calculations involving two components. You can think of this activity as a combination of a System Definer and an Equilibrium Calculator, but designed to simplify setting up and performing calculations on binary systems.

The Binary Calculator relies on some specifications that are not supported by all databases. You need a specially designed database for the Binary Calculator such as the TCBIN database.



For an example of how a Binary Calculator can be used in a project, see example 3 in [Graphical Mode Example Collection](#) on page 9.

## Configuration Window

The following shows the **Configuration** window of a **Binary Calculator** activity.

## Configuration Settings

The table lists the available settings to configure before performing the calculation.





Also see [Creating Activities and Successors on page 29](#) for a list of possible successors and predecessors for this activity.

Setting	Description
Select database	Select a database that contains specifications dedicated to the Binary Calculator.
Elements (periodic table)	In the periodic table, select the two elements that make up the components of the system.
Phases and Phase Constitution	This tab is the same as for a <a href="#">System Definer on page 54</a> . See <i>Phases and Phase Constitution</i> for an example.
Data Sources	This tab is the same as for a <a href="#">System Definer on page 54</a> . See <i>Data Sources</i> for an example.
Description	This tab is the same as for a <a href="#">System Definer on page 54</a> . See <i>Description</i> for an example.
<b>Calculation Type</b>	
Phase diagram	Select to perform a mapping calculation. Click <b>Calculate Phase Diagram</b> to plot the results.
Gibbs energy curves	Select the <b>Temperature</b> and click <b>Calculate Gibbs Energy Curves</b> to calculate at a constant temperature over the whole composition range.
Activity curves	Select the <b>Temperature</b> and click <b>Calculate Activity Curves</b> to calculate at a constant temperature over the whole composition range.
Phase fractions	Select the <b>Mole fraction</b> and click <b>Calculate Phase Fractions</b> to calculate as a function of temperature at a constant composition.

## Ternary Calculator

A Ternary Calculator is used for some calculations involving three components. You can think of this activity as a combination of a System Definer and an Equilibrium Calculator, but designed to simplify setting up and performing calculations on ternary systems.



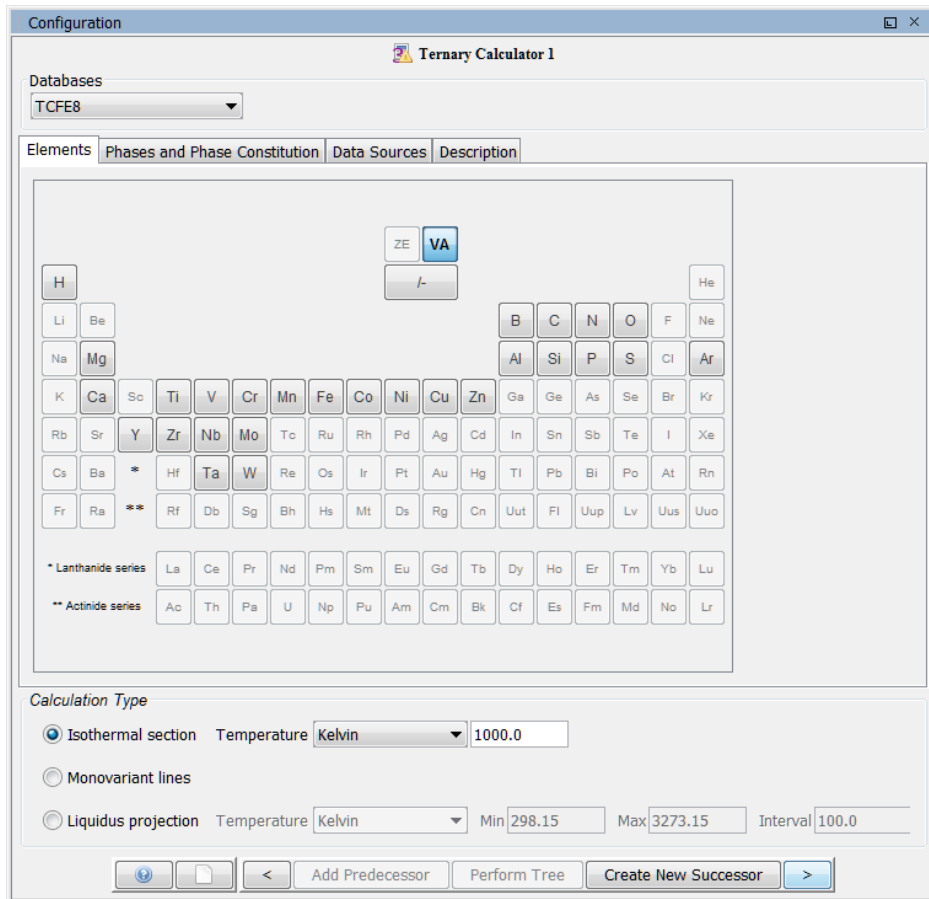
For an example of how a Ternary Calculator is used in a project, see example 4 in [Graphical Mode Example Collection on page 9](#).



Also see [Creating Activities and Successors](#) on page 29 for a list of possible successors and predecessors for this activity.

## Configuration Window

The following shows the Configuration window of a Ternary Calculator activity:



## Configuration Settings

The table lists the available settings that must be configured before performing the calculation.

Setting	Description
Select database	Select a database that contains specifications dedicated to the Ternary Calculator.
Elements (periodic table)	In the periodic table, select the three elements that make up the components of the system.

Setting	Description
Phases and Phase Constitution	This tab is the same as for a <i>System Definer</i> on page 54. See <i>Phases and Phase Constitution</i> for an example.
Data Sources	This tab is the same as for a <i>System Definer</i> on page 54. See <i>Data Sources</i> for an example.
Description	This tab is the same as for a <i>System Definer</i> on page 54. See <i>Description</i> for an example.
Calculation Types	
Isothermal section	Select the <b>Temperature</b> at which the ternary system is calculated for the whole composition range.
Monovariant lines	The variation of the liquid compositions with temperature is calculated.
Liquidus projection	Select the <b>Temperature</b> range ( <b>Min</b> and <b>Max</b> ) and an <b>Interval</b> . The projection liquid surface and the monovariant lines are calculated over the given temperature range.

## Scheil Calculator

The Scheil Calculator activity is used to perform simulations of *Scheil (Scheil-Gulliver) solidification processes*. By default, a Scheil calculation results in an estimation of the solidification range of an alloy. The calculation is based on the assumption that the liquid phase is homogeneous at all times and that the diffusivity is zero in the solid. However, it is possible to disregard the latter assumption for selected components.

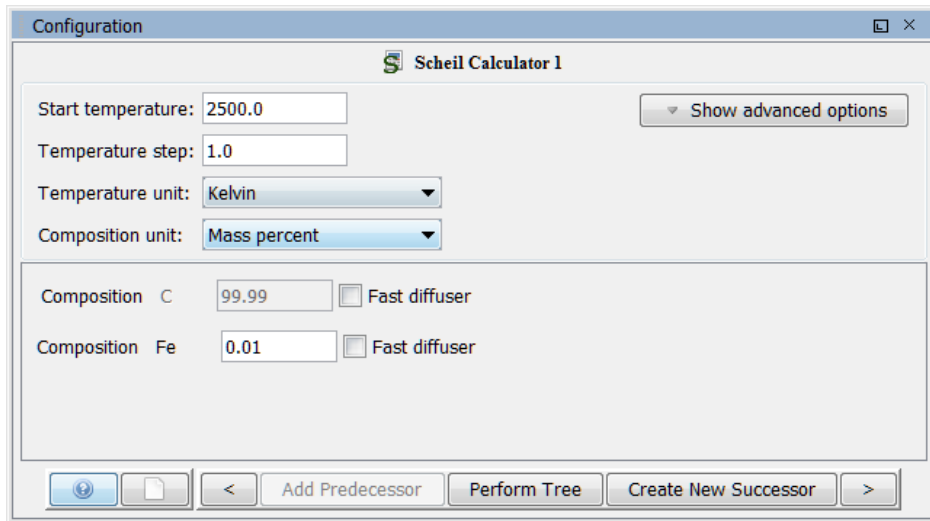
By default, a Plot Renderer successor has the default plot axes **Mole fraction of solid** (X-axis) and **Temperature Celsius** (Y-axis). When these default axes are used in the Plot Renderer, the results of normal equilibria calculations are automatically plotted in the same diagram as the Scheil calculations.



See example 8 in *Graphical Mode Example Collection* on page 9.

## Configuration Window

The main **Configuration** window of a **Scheil Calculator** activity is shown below and listed in the table. These settings must be configured before performing the calculation.



## Configuration Settings

Setting	Description
Start temperature	Enter a <b>Start temperature</b> that is higher than the liquidus temperature of the alloy, in other words, the temperature at which the alloy is completely melted.
Temperature step	Enter a <b>Temperature step</b> . Decreasing the temperature step increases the accuracy, but the default value is usually adequate.
Temperature unit	Select the <b>Temperature unit</b> : Kelvin, Celsius or Fahrenheit.
Composition unit	Select the <b>Composition unit</b> : Mass percent, Mole percent, Mass fraction or Mole fraction.
Composition	This is based on what is entered in the <a href="#">System Definer on page 54</a> .
Fast diffuser	Click to select the <b>Fast diffuser</b> check box to allow redistribution of this component in both the solid and liquid parts of the alloy.

## Scheil Calculator Advanced Options and Settings

Additional advanced settings are available as shown below and in the table:

Click **Show advanced options** to open this configuration window:

## Scheil Calculator Advanced Settings

Setting	Description
Global minimization	By default the <b>Global minimization</b> check box is not selected. Click to select it to perform a global minimization test when an equilibrium is reached. This costs more computer time but the calculations are more robust.
Allow BCC→FCC	By default the <b>Allow BCC → FCC</b> check box is not selected. Select the check box to allow transformations in the solidified part of the alloy caused by each of the components specified to be a <i>fast diffuser</i> . It is recommended that you only select this for steels.
Liquid phase	The default in the list is the <b>Liquid phase</b> already defined in the database.
Terminate on	Enter a value to terminate the calculation on the <b>Fraction of liquid phase</b> or at a specific <b>Temperature</b> .



Also see [Creating Activities and Successors](#) on page 29 for a list of possible successors and predecessors for this activity and [Scheil Simulations](#) on page 144 in the Console Mode section.

---

## The Console Mode Interface

The following is an introduction to the Console Mode's user interface and the command line prompt.



Also see [The Graphical Mode Interface](#) on page 26 for information about that mode.

In this section:

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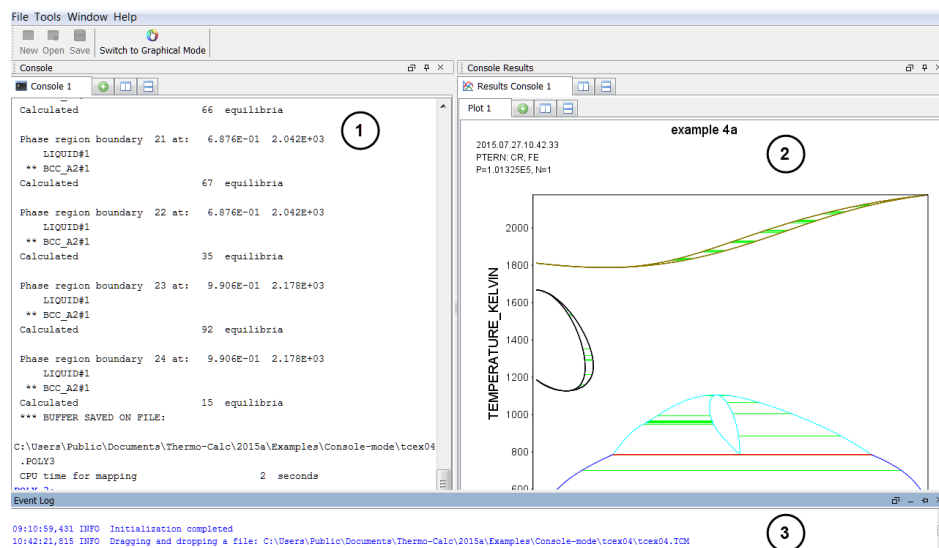
<i>The Console Mode Layout</i> .....	112
<i>Console Window</i> .....	113
<i>Editing the Default Console Directory</i> .....	114
<i>Console Mode Results Window</i> .....	116
<i>Event Log Window</i> .....	116
<i>Console Mode Workflow</i> .....	117
<i>Performing Calculations in Console Mode</i> .....	118
<i>Using the Command Line Prompt</i> .....	119
<i>Moving Between Modules and Submodules</i> .....	119
<i>Entering Command Names or Abbreviations</i> .....	120
<i>Specifying Parameters</i> .....	121
<i>Wild Card Characters</i> .....	122
<i>Controlling Console Output</i> .....	123
<i>Command History</i> .....	123
<i>Log, Macro and Workspace Files</i> .....	123
<i>Log Files</i> .....	124
<i>Macro Files</i> .....	124
<i>Workspace Files</i> .....	126
<i>Main Menu Commands</i> .....	127
<i>Defining a System in Console Mode</i> .....	127

---

## The Console Mode Layout

By default the first time you launch Thermo-Calc it opens in Graphical Mode. After this, the mode defaults to the most recent one. You can switch back and forth between modes. To open the Console Mode interface, click **Switch to Console Mode** on the toolbar.

### The Console Mode User Interface

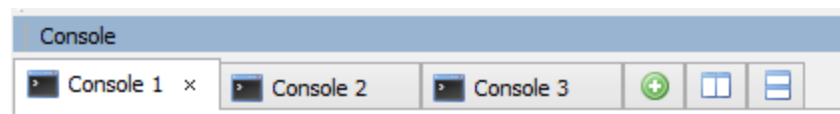


The currently selected window is called the *active* window. This has a darker title bar than the other windows. The windows are:

1. **Console**, with a **Console 1** tab.
2. **Console Results**, with a **Results Console 1** tab as well as a sub-tab (**Plot 1**), which is what is displayed in the window in the figure.
3. **Event Log**, which is the active window in this example.

### Console Tabs

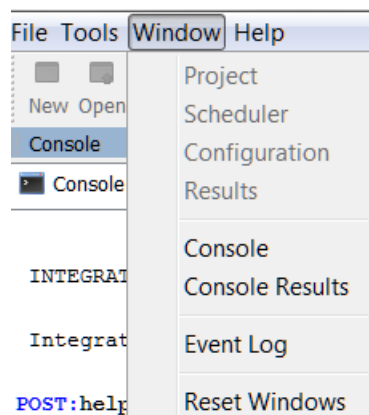
By default, the tabs are side-by-side:



You can toggle to view the tabs top-to-bottom/stacked (click the button) and back to side-by-side (click the button) or the button.

### Open Console Windows



Open a specific window from the **Window** main menu, or select **Reset Windows** to return to the default window layout.



## Console Window

By default the Console window is on the left-hand side of the console. This is where you enter commands. The window can have several Console tabs.

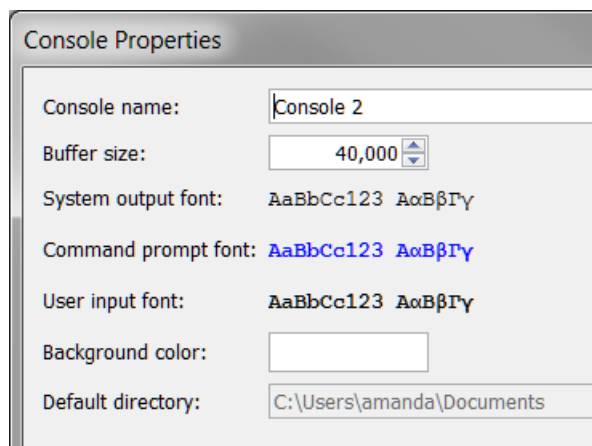
To open and close Console tabs:

- To open (or add), click the  button, press <Ctrl+T> when the Console window is active, or right-click a tab header and select **New Console**.
- To close, click the  button, press <Ctrl+W> or <Ctrl+F4>, or right-click the tab header and select **Close**.
- To close all tabs except one, right-click the header of the tab you want to keep and select **Close Other**.
- To close all tabs and open a new one, right-click the header of any tab and select **Close All**.

You can change the tab name, font and colours for an individual Console tab by right-clicking its header and selecting **Properties**.



## Console Properties Window



## Editing the Default Console Directory

You can add a startup parameter to a shortcut when launching Thermo-Calc on any of the platforms. When you launch the revised shortcut, the file path is set to a user-defined default directory. An example of why you might want to have a custom directory path is if you use batch projects or if you have macro files for batch jobs. The custom directory file path can also be viewed from within Console Mode.

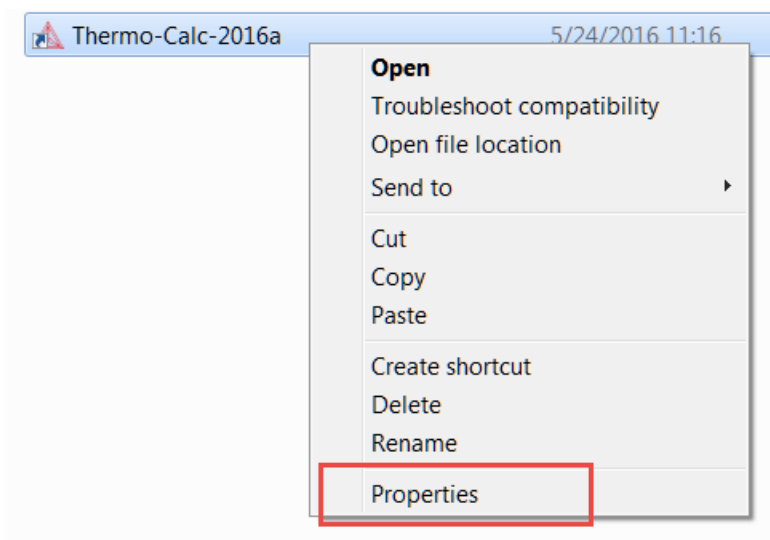


The shortcut is only valid throughout the existing session; it is not saved as a default. Each time you want to use this file path you must launch Thermo-Calc from the customized shortcut.

The following uses Windows for the example.

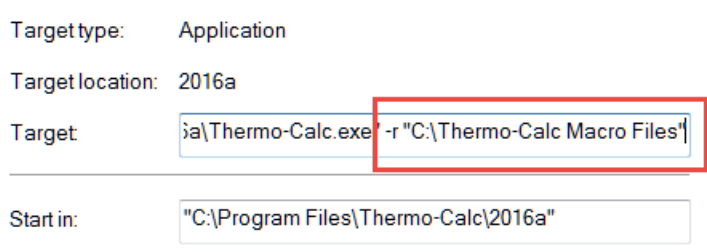
### Setting up the Default Console Directory

1. Right-click a shortcut to Thermo-Calc and click **Properties**.



2. In the **Thermo-Calc 2016a Properties** dialog, **Target** field, add the following to the end of the string: `-r` plus the *“path to the default directory”*. Include a space between the `-r` and path, and use quotation marks around the full file path. A simple example:

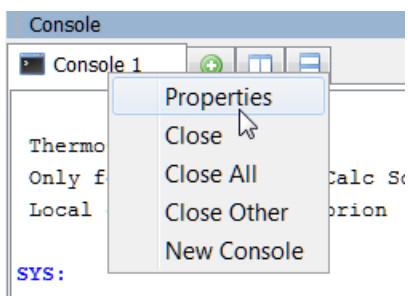
**-r “C:\Thermo-Calc\_Macro\_Files”**



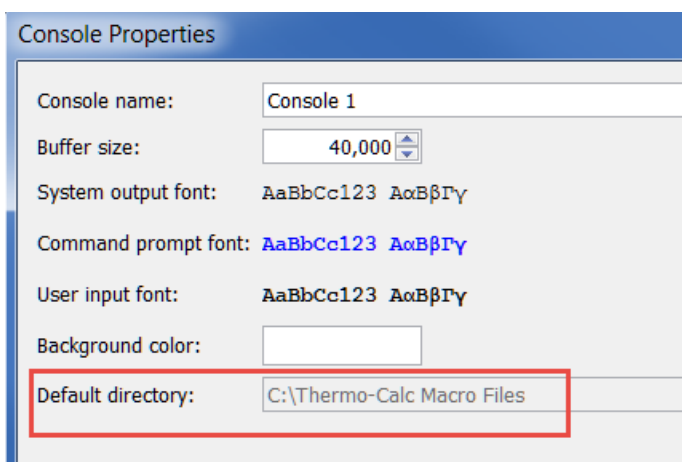
3. Click **Apply** and **OK**.
4. Launch Thermo-Calc from the shortcut where you added the parameter. You can confirm that it is set correctly from within Thermo-Calc.

### Viewing the File Path in Thermo-Calc

1. Launch Thermo-Calc from the short cut where you added the parameter.
2. In Console Mode, right click the **Console** window and choose **Properties**.




3. In the **Console Properties** window the **Default directory** section displays the custom file path.



## Console Mode Results Window

By default, the Console Results window is on the right-hand side of the screen. This is where plotted diagrams display. Each Console has its own Results tab in the Results window. All the plots and tables generated are presented in the Results tab.

- To open new **Plot** tabs press <Ctrl+Shift+T> or click the add  button.
- To open a new Plot tab for the currently active Console tab, press <Ctrl+Shift+T>. To close the Plot tab, press <Ctrl+Shift+W> or <Ctrl+Shift+F4>.

## Event Log Window

By default the Event Log window is collapsed (closed). It includes important information about the commands that run and are completed, including error messages. Click once to toggle it open and closed.

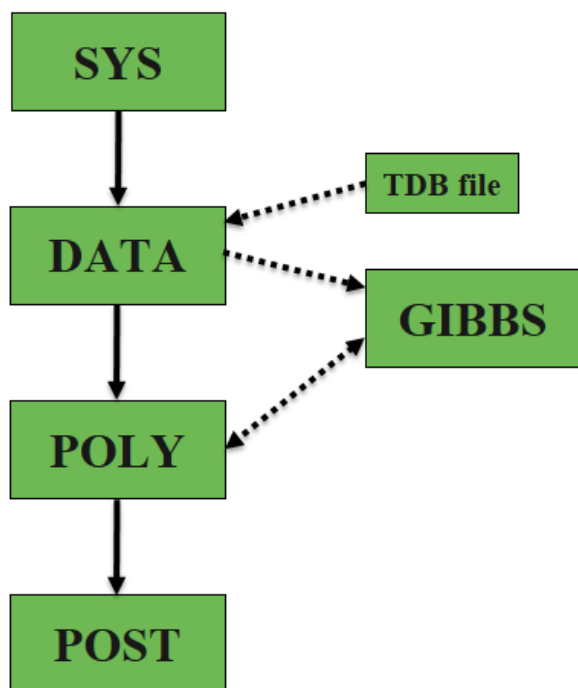
## Console Mode Workflow

Working with Thermo-Calc involves moving between different modules. The workflow differs depending on the type of calculation:

- If you want to perform a calculation using the POLY module, you typically first retrieve thermodynamic data in the DATA module, perform the calculation in POLY, and visualize the results in the POST module. It is possible to define a system directly in POLY using [DEFINE\\_MATERIAL on page 147](#) and [DEFINE\\_DIAGRAM on page 144](#).
- If you want to calculate and plot a diagram using a response-driven module, such as POTENTIAL or SCHEIL, then you can go directly to that module. Response-driven modules prompt you to go through the steps to do the calculation and the required post-processing. These modules include BIN, TERN, POTENTIAL, POURBAIX, and SCHEIL. You typically end up in the POST module after having used a response-driven module. In the POST module you can modify the plots and save the diagram.
- If you want to tabulate a chemical substance, phase, or reaction, go directly to the TAB module.

### Typical POLY Module Workflow

The following represents the typical workflow when you perform calculations in the POLY module. The solid arrows represent your typical movements between the modules. The dashed arrows represent the movement of data within Thermo-Calc.



The basic workflow is:

1. You are in the **SYS** module when you start Thermo-Calc in Console Mode.
2. In the **DATA** module define the system. Before performing a calculation, you must define the system and retrieve thermodynamic data. The data is retrieved from a data-base file (\*.TDB or \*.TDC).
3. The data needed to describe a system is then sent to the **GIBBS** module. This data is accessed by the **POLY** module when you instruct it to perform calculations.
4. In the **POLY** module, perform the calculations.
  - In POLY, the conditions are set for an equilibrium calculation (temperature, pressure, system composition, etc.), then an equilibrium calculation is done.
  - If you want to make a property or phase diagram, you set the conditions for a stepping or mapping operation and perform that operation.
  - This generates data that can be used to plot a property diagram (if a stepping operation is performed) or a phase diagram (if a mapping operation is performed).
5. In the **POST** module plot and visualize your data.
  - If a stepping or mapping operation is performed, then you can go to the POST module and plot a property or phase diagram.
  - The diagram can be plotted quickly using default settings, but you can also modify which variables to plot of the diagram axes and change the appearance of the diagram.
  - You can save the diagram either as a plain text file with data about all the coordinates or as an image file.

## Performing Calculations in Console Mode

Calculations can be performed either in the POLY module, or using some of the response-driven modules designed to perform specific types of calculations.

*About Equilibrium Calculations on page 131* describes generally how to calculate and plot *Property Diagrams* and *Phase Diagrams*. To calculate and plot a property diagram or a phase diagram, you must first calculate an equilibrium.

Additional sections of use include *About Scheil Simulations on page 145*, *T0 Temperature Simulations on page 151*, *About Paraequilibrium on page 154*, *About Potential Diagrams on page 158*, and *About Aqueous Solutions on page 162*. Also search the online help or see *TABULATION\_REACTION Commands on page 245* and *POLY\_3 Commands on page 117* in the *Thermo-Calc Console Mode Command Reference*.

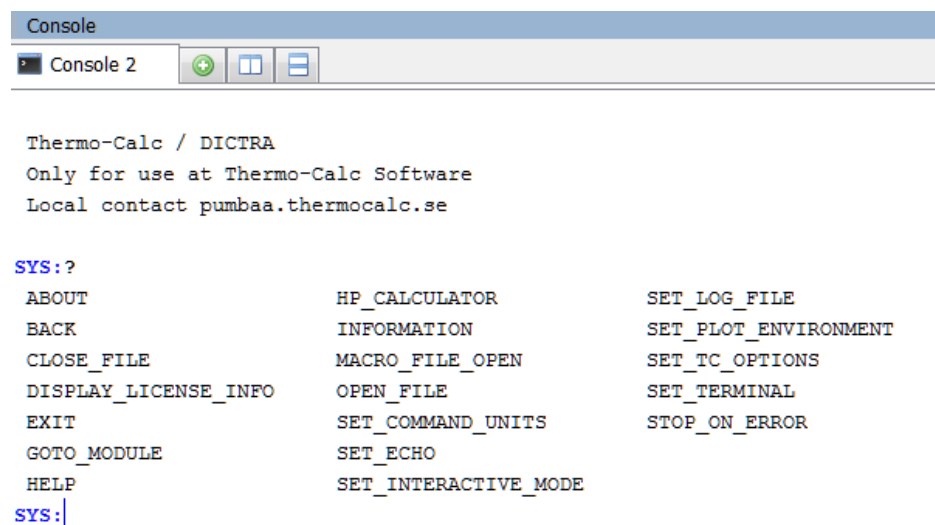
## Using the Command Line Prompt

The command line prompt in the Console window tells you which module you are currently in. When Thermo-Calc is first opened in Console Mode, you are in the SYS module, which is indicated with the command line prompt `SYS`.

To use Console Mode, you type in commands at the command line prompt. The available commands depend on which module you are in. You can list the commands by typing `?` at the prompt and then press <Enter>.

- [Moving Between Modules and Submodules below](#)
- [Entering Command Names or Abbreviations on the next page](#)
- [Specifying Parameters on page 121](#)
- [Wild Card Characters on page 122](#)
- [Controlling Console Output on page 123](#)
- [Command History on page 123](#)

### Available SYS Module Commands



```

Console
Console 2

Thermo-Calc / DICTRA
Only for use at Thermo-Calc Software
Local contact pumbaa.thermocalc.se

SYS:?
ABOUT          HP_CALCULATOR      SET_LOG_FILE
BACK            INFORMATION        SET_PLOT_ENVIRONMENT
CLOSE_FILE      MACRO_FILE_OPEN     SET_TC_OPTIONS
DISPLAY_LICENSE_INFO OPEN_FILE           SET_TERMINAL
EXIT            SET_COMMAND_UNITS   STOP_ON_ERROR
GOTO_MODULE     SET_ECHO
HELP            SET_INTERACTIVE_MODE
SYS:|
  
```

## Moving Between Modules and Submodules

To go to a specific module, you typically use `GOTO_MODULE` (or just `GOTO`) followed by the name of the module. For example, to go to the DATA module, type `GOTO DATA`.

The exceptions are the submodules POST and ED-EXP:

- To go to the POST module, you must enter the POST command from within the POLY module or DICTRA module (if you have the add-on license).

- To go to [Experimental Data Files on page 36](#), you must enter the ED-EXP command from within the PARROT module.

To go back to the previous module type `Back`. For example, if you are in the DATA module and entered it from the SYS module, when you type `Back`, you return to the SYS prompt. This command is also available to exit from the submodules POST and ED-EXP.



Without a valid Thermo-Calc license, you cannot leave the SYS module. To enter the DICTRA and DIC\_PARROT modules, you also need a valid Diffusion Module (DICTRA) license key.

## Entering Command Names or Abbreviations

The name of a command typically consists of terms linked with underscores, for example, [LIST\\_EQUILIBRIUM on page 156](#). Note the following:

- UPPER or lower case letters are OK.
- Hyphens (-) instead of underscores (\_) are OK, e.g. LIST-EQUILIBRIUM.
- You can abbreviate commands as long as it is unambiguous, e.g. when more than one command begins with LIST\_, you need to type the next letter or word to distinguish between the commands.
- Each word can be abbreviated e.g., L\_E for LIST\_EQUILIBRIUM.

### Command Names and Abbreviations Examples

These are examples of how you can abbreviate commands at the command line prompt.

Command name	Abbreviation
CALCULATE_EQUILIBRIUM	C-E
CALCULATE_ALL_EQUILIBRIA	C-A
LIST_EQUILIBRIUM	L-E
LIST_INITIAL_EQUILBRIUM	LI-I-E
LOAD_INITIAL_EQUILBRIUM	LO-I-E
LIST_PHASE_DATA CBCC	L-P-D CBC
LIST_PHASE_DATA CEMENTITE	L-P-D CEM
SET_ALL_START_VALUES	S-A-SS-AL
SET_AXIS_VARIABLE 1 X(FCC,FE) 0 0.89 0.025	S-A-V 1 X(F,FE) 0 .89 .025

Command name	Abbreviation
SET_START_CONSTITUENT	S-S-C
SET_START_VALUE	S-S-V
SET_AXIS_PLOT_STATUS	S-A-P
SET_AXIS_TEXT_STATUS	S-A-T-SS-A-TE
SET_AXIS_TYPE	S-A-TY
SET_OPTIMIZING_CONDITION	S-O-C
SET_OPTIMIZING_VARIABLE	S-O-V
SET_OUTPUT_LEVEL	S-O-LS-OU

## Specifying Parameters

Running a command typically requires that several parameter values are specified, which can be done directly in the command line after the command name. For example, to set an axis variable for a stepping or mapping operation, enter:

```
SET_AXIS_VARIABLE 1 X(FCC,FE) 0 0.89 0.025
```

You can also use SET\_AXIS\_VARIABLE and press <Enter>. At the command line prompt, you then specify the parameters one at a time.

On all command lines, you can enter a question mark (?) for help. For some parameters, enter two question marks (??) for more detailed information.

### Default Parameters Values

When you are requested to specify a parameter, Thermo-Calc usually suggests an appropriate default value, which is displayed at the prompt between two slash signs (/). For example, this prompt means the default answer is `TERMINAL`:

```
OUTPUT FILE /TERMINAL/:
```

Press <Enter> to accept the default.

If you specify some parameters directly after the command name, then you can still choose to accept default values for some parameters.

To accept the default value for a parameter, type a comma (,) instead of a value for that parameter. For the comma to be interpreted correctly, type a blank space on each side of the comma. However, if you accept the default values for several parameters that follow each other, then the commas can be typed in without blank spaces separating them: (, , ,) is interpreted in the same way as (, , ,).

For some commands and parameters, Thermo-Calc treats the values previously assigned as default values if the command is used again. For example, if the first stepping or mapping axis variable is



specified as:

```
SET_AXIS_VARIABLE 1 X(FCC,FE) 0 0.89 0.025
```

Then if you want to change a parameter value for this axis variable, type:

```
SET_AXIS_VARIABLE 1 , 0.1 , , ,
```

This changes the minimum value from 0 to 0.1 at which a stepping or mapping operation halts. The other parameter values remain the same. Consequently, what is typed is equivalent to:

```
SET_AXIS_VARIABLE 1 X(FCC,FE) 0.1 0.89 0.025
```

## Wild Card Characters

You can sometimes use the asterisk (\*) as a wild card character to, for example, refer to all components, phases, or species, when showing calculated properties in the POLY module, or when you set axis variables for plotting diagrams in the POST module.

When showing calculated properties in the POLY module, you can also use the dollar sign (\$) to refer to all stable phases.



For activity and/or chemical potential properties, the \* and \$ normally do not work properly as wild card characters.

## Wild Card Character Examples

These are examples of the wild card characters you can use to search commands at the command line prompt.

Command	Action
SHOW_VALUE B(*)	Lists mass (gram) of all components in the system.
SET_AXIS_VAR Y B(*) *	Sets mass (gram) of all components in the system as Y-axis variable.
SHOW_VALUE MUR(*)	Lists chemical potentials of all components in the system.
SET_AXIS_VAR Y ACR(*) *	Sets activities of all components in the system as Y-axis variable.
SHOW_VALUE HM(*).T	Lists heat capacities of all phases.
SET_AXIS_VAR Y GM(*) *	Sets molar Gibbs free energies of all phases as Y-axis variable.
SHOW_VALUE TC(\$)	Lists curie temperature of all stable phases.
SHOW_VALUE W(*,*)	Lists mass fractions of all components in all phases.
SHOW_VALUE W(\$,*)	Lists mass fractions of all components in all stable phases.

Command	Action
SHOW_VALUE W(FCC,*)	Lists mass fractions of all components in the FCC phase.
SHOW_VALUE W(*,FE)	Lists mass fractions of the Fe component in all phases.
SHOW_VALUE W(\$,FE)	Lists mass fractions of the Fe component in all stable phases.
SHOW_VALUE Y(*,*)	Lists site fractions of all species in all sublattices of all phases.
SHOW_VALUE Y(\$,*)	Lists site fractions of all species in all sublattices of all stable phases.
SHOW_VALUE Y(*,*)	Lists site fractions of all species in all sublattices of all phases.

## Controlling Console Output

In response to a command Thermo-Calc may display a lot of text in the Console window.

- To pause the text on printing press <Ctrl+S>.
- To resume the printing on screen, press <Ctrl+Q>.
- When Thermo-Calc is performing a mapping operation, the results are continuously printed in the Console window. To terminate the calculation of the current region of the mapping and stop the output, press <Ctrl+C>.

## Command History

- To scroll through the last twenty commands used, type two exclamation marks (!!) and press <Enter>.
- To repeat the last n commands, type ! followed by the number of previous commands to be executed again.
- To scroll through previous performed commands, use the Up (↑) or Down arrow (↓) keys.
- To read more information about the command history functionality in Thermo-Calc, type ! ? at the command line prompt.

## Log, Macro and Workspace Files

In Console Mode, Thermo-Calc uses different kinds of files, including:

- *Log Files on the next page* (\*.LOG)
- *Macro Files on the next page* (\*.TCM or \*.LOG)

- POLY [Workspace Files on page 126](#) (\*.POLY3),
- [Experimental Data Files on page 36](#) (\*.EXP)



Also see the [Data Optimization User Guide on page 1](#).

- The GIBBS module uses a workspace file (\*.GES5). See [GIBBS\\_ENERGY\\_SYSTEM Commands on page 42](#)
- The PARROT module uses files with the suffixes \*.PAR and \*.POP. See [PARROT Commands on page 86](#)

## Log Files

Log files are plain text files used to save a sequence of commands. Log files can be edited in a text editor.

- To start saving your input into such a file, use SET\_LOG\_FILE in the SYS module, followed by the name of the file that you want to save your command sequence to.
- If you want to save the output in the log file as well, use SET\_ECHO before the SET\_LOG\_FILE command. Doing this is useful if you want use the log file later as a macro file.



See [SYSTEM\\_UTILITIES Commands on page 239](#) in the *Thermo-Calc Console Mode Command Reference*.

## Macro Files

Macro files are plain text files used to save a sequence of commands that can be loaded and executed. Macro files can be edited in a text editor.

### Macro File Commands



Also see Example 12 in [Console Mode Example Collection on page 14](#).

Action	Command	Description and Comments
To load a macro file	In the SYS module, <a href="#">MACRO_FILE_OPEN on page 5</a> followed by the name of the macro file.	Thermo-Calc starts the command sequence that the file contains.
Regain control of the console	<a href="#">SET_INTERACTIVE on page 8</a>	End a macro file with this command to have control of the Console returned to you.

Action	Command	Description and Comments
Add comments to a macro file	Start a line with @@, or enclose it between an @ (-line and a @)-line.	When lines are enclosed the software ignores them when running the macro.
Open a macro file	MACRO_FILE_OPEN	When creating the log file, you can make a macro file load up to five other macro files.
Nest macro files inside of each other	MACRO_FILE_OPEN SET_INTERACTIVE	If a nested macro file ends with SET_INTERACTIVE, then Thermo-Calc resumes with the higher-level macro file at the command immediately following the MACRO_FILE_OPEN command that loaded and executed macro file that has just been terminated. If a nested macro file doesn't end with SET_INTERACTIVE (but with an end-of-file character), then the console shuts down and the macro is stopped.

## Macro File Control Characters

The @? character allows you to make a macro interactive by allowing input. At the @? character, which is placed where a parameter value or argument is normally put, Thermo-Calc prompts to input the value of a parameter or argument. You can enter a string immediately following the @? character. This string is presented to the user when prompted to enter the parameter value or argument. The entered value is used by Thermo-Calc as input to the command in question. For example, you can request the user to specify the temperature range of a stepping calculation by entering the following in a macro file:

```
SET_AXIS_VARIABLE 1 T @?Low-temperature-limit: @?High-temperature-limit:
```

You can also use up to nine variables in your macro file and prompt the user to enter values that can be assigned to these variables. Use the @#n character when you want to prompt the user to provide a value to the variable, where the n is a digit between 1 and 9. You can then use this value by with the ##n character. For example, you can request the user to provide the first element of a system by entering the following in the macro file:

```
@#3First-element?
```

You can then use this variable with the entering the character ##3 later in the macro file. For example, you can write:

```
SET_AXIS_VARIABLE 1 x(##3) 0 1,,,
```

Finally, there is the @& pause character. Thermo-Calc pauses and waits for input from the user when this pause character is read from a macro file. Inserting pause characters is useful if you want to allow the user to monitor what is happening when Thermo-Calc is running the macro.

## Response-Driven Modules and Macros

Macro files that are created while you use a *response-driven module* begin with the module-entering command (for example, `Goto_Module Scheil`) followed by a number of lines with responses to the module's questions and requests. The file terminates with the commands [POST on page 160](#) or [SET\\_INTERACTIVE on page 8](#) (this command gives you back control of the Console). An empty line cannot be edited with any input rather than the default answer (to a specific question). Comment lines, commands to open other macro files, pause characters or input-controlling characters cannot be inserted between these empty lines (otherwise the response-driven module cannot be executed properly).

## Workspace Files

You can save all the data in your current workspace by first using `SAVE_WORKSPACES`. This command is available in the POLY, GIBBS and PARROT modules. The workspace has all the settings specified and the result of any stepping or mapping operations performed after using `SAVE_WORKSPACES`. Consequently, the command opens a workspace in which all data is saved which is generated after the `SAVE_WORKSPACE` command is executed. The saved data includes original and modified thermodynamic data, the last set of conditions and options, and calculation results.

To load the data and calculation results of a workspace file, use the `READ_WORKSPACES` command available in the POLY module. The file can be used for calculation in POLY, visualization in POST, or data

manipulation in GIBBS. You are also given the option in the POURBAIX and SCHEIL modules to open a previously saved workspace file. This allows you to make new POURBAIX or SCHEIL calculations on the same chemical system as before but with different temperature, pressure, and composition conditions, or to plot new property diagrams based on the previous calculations.

## Main Menu Commands

The **File** menu and toolbar are reserved for Graphical Mode. In Console Mode you use commands to access these menu options. The **Tools**, **Window** and **Help** menus are described in [Main Menu and Toolbar on page 32](#). If there is an equivalent command, it is listed in the table below.

### Console Mode Main Menu Commands

Option	Command
Open files	In Thermo-Calc, drag and drop the file into the Console window. In the SYS module: <a href="#">MACRO_FILE_OPEN on page 5</a> In the SYS module: <a href="#">OPEN_FILE on page 241</a>
Save (workspace)	This command depends on the module you are in. Type ? at the prompt to look for a command such as <a href="#">SAVE_GES_WORKSPACE on page 84</a> (GIBBS module)
Exit	In any module: EXIT
Close	In the SYS module: <a href="#">CLOSE_FILE on page 240</a>
Display license info	In the SYS module: <a href="#">DISPLAY_LICENSE_INFO on page 240</a>

## Defining a System in Console Mode

*Defining a system* means to select the chemical components and to retrieve thermodynamic data about those components from an appropriate database in order to do the calculations. You use database(s) with thermodynamic data and then define what system elements as components. Once the system is defined, you retrieve the system's thermodynamic data from the database(s).

- If you use a *response-driven module* to perform your calculation, such as BIN or POURBAIX, then the module prompts you to select database(s) and define the system.
- When doing calculations in the POLY module, you typically have to manually select databases and define the system in the DATA module. However, it is also possible to define the system directly in POLY using [DEFINE\\_MATERIAL on page 147](#) and [DEFINE\\_DIAGRAM on page 144](#).



Also see [DATABASE\\_RETRIEVAL Commands](#) on page 11 in the *Thermo-Calc Console Mode Command Reference*.

## How to Define a System in Console Mode

1. Go to the DATA module. At the `SYS` prompt, use `GOTO_MODULE` and enter `Data`.
2. Change the default database unless you directly specify the name of the database as a parameter to the command. Type `SWITCH_DATABASE` and follow the prompts.

The second part of the command prompt indicates the current default database. For example, if the prompt is `TDB_TCFE8`, then the current database is TCFE8.

3. Use `DEFINE_ELEMENTS` followed by a list of the elements that you want in your system. (To list the elements that are available in your current database, use `LIST_DATABASE` and choose `Elements`). For example, if you want to have Fe and C in your system, type:

```
DEFINE_ELEMENTS Fe C
```

4. Use `REJECT` and choose `Phases` if you want to avoid retrieving any phases from the database. (To list the phases that are available in your current database, use `LIST_DATABASE` and choose `Phases`. To list the phases that can form in the defined system, use `LIST_SYSTEM` and choose `Constituent`.) For example, if you do not want the graphite phase to be retrieved, you type:

```
REJECT PHASES GRAPHITE
```

If the number of phases to include is much lower than the total number of phases, then it can be convenient to first `Reject Phases *` and then restore the phases to include using `Restore Phases`.

5. Use `GET_DATA` to search the database and send the thermodynamic data about your system to the GIBBS workspace.

At this point you can proceed to the POLY module (with `GOTO_MODULE POLY`). However, you may want to add elements, phases and species to the GIBBS workspace from other databases. If so, then proceed to the next step.

6. Use `APPEND_DATABASE` to select the (additional) database from which you want to retrieve data. This command works exactly in the same way as the `SWITCH_DATABASE` command, with the exception that it does not reinitialize the DATA module and the GIBBS workspace, but instead appends or replaces the data that has already been retrieved with new data from the additional database.
7. Define your elements and specify whether to reject and restore any phases. Do this in

exactly the same way when using the SWITCH\_DATABASE command (see steps 2 and 3).

8. Use GET\_DATA to search the database and add the thermodynamic data to the data that already exists in the GIBBS workspace.
9. Use APPEND\_DATABASE again if you want to add data from yet another database. When you have retrieved all the data you need, you can proceed to the POLY module.



---

# Equilibrium Calculations

In this section:

---

<i>About Equilibrium Calculations .....</i>	<i>131</i>
<i>Calculating an Equilibrium .....</i>	<i>133</i>
<i>Calculating an Equilibrium with a Fixed Phase .....</i>	<i>134</i>
<i>Calculating an Equilibrium with Suspended or Dormant Phases .....</i>	<i>134</i>

## About Equilibrium Calculations

An equilibrium describes what the composition of the end state of a system is, given a full specification of state variables such as temperature, pressure, initial composition, system size, etc. An equilibrium calculation is normally done in POLY-3 according to the *Global Minimization Technique*, which ensures that the most stable minimum under the specified conditions is computed.

For an equilibrium calculation to be performed, the state variables must all be set as conditions for the calculations. Such conditions include, for example, temperature, pressure, and system composition. When you calculate an equilibrium in the POLY module, you have to set these conditions manually.

### Setting Conditions

Setting a condition normally involves giving a single state variable a specific value. For example, you can set the temperature to 1273.5 Kelvin ( $T=1273.5$ ). Alternatively, setting a condition can involve giving a linear expression with more than one state variable a specific value. For example, you can set the mole fraction of the S component to be the same in the liquid and the pyrrohotite phases ( $X(\text{LIQ}, S) - X(\text{PYRR}, S) = 0$ ).

The number of state variables that need to set is determined by the *Gibbs Phase Rule*. Typically, the state variables to give values to are:

- temperature (in K)
- pressure (in Pascal)
- system size in number of moles (in mole) or mass (in grams)
- the fraction of each component (in number of moles or mass)

If you fix the phase of the equilibrium and all but one of the state variables, you can discover the value of the other state variable at equilibrium.

It is possible to specify a set of conditions that does not have any equilibrium and the program detects this by failing to reach equilibrium during the calculation.

### State Variables for Setting Conditions

The following table lists some of the available state variables you can use to set conditions:

State Variable	SET_CONDITION Parameter
temperature in the system (in K)	T
pressure in the system (in Pascal)	P
system size (mole number in moles)	N
system size (mass in grams)	B

State Variable	SET_CONDITION Parameter
number of moles of a component in the system	N(<component>)
mole fraction of a component in the system	X(<component>)
mass fraction of a component in the system	W(<component>)
activity of a component in the system	ACR(<component>)
chemical potential of a component in the system	MUR(<component>)
mole fraction of a component in a phase	X(<phase>,<component>)
mass fraction of a component in a phase	W(<phase>,<component>)
activity of a species referred to a phase at ambient temperature and pressure	ACR(<species>,<phase>)
chemical potential of a species referred to a phase at ambient temperature and pressure	MUR(<species>,<phase>)
enthalpy in the system (in J)	H
enthalpy of a phase (in J/mol)	HM(<phase>)

### Equilibrium Information Example

```

POLY_3:l-e
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium =      1, label A0 , database: TCFE7

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

Temperature 1000.00 K ( 726.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 5.36552E+01
Total Gibbs energy -4.07975E+04, Enthalpy 2.41176E+04, Volume 7.21740E-06

Component      Moles      W-Fraction Activity Potential Ref.stat
C               5.0000E-02  1.1193E-02 2.1816E-01 -1.2659E+04 SER
FE              9.5000E-01  9.8881E-01 6.1895E-03 -4.2279E+04 SER

BCC_A2                      Status ENTERED      Driving force 0.0000E+00
Moles 9.5069E-01, Mass 5.3063E+01, Volume fraction 9.6312E-01 Mass fractions:
FE 9.99844E-01 C 1.55514E-04

GRAPHITE                      Status ENTERED      Driving force 0.0000E+00
Moles 4.9313E-02, Mass 5.9230E-01, Volume fraction 3.6881E-02 Mass fractions:
C 1.00000E+00 FE 0.00000E+00

```

## Calculating an Equilibrium

This topic explains how to calculate an equilibrium in POLY. To calculate an equilibrium means to calculate the equilibrium composition of your system, given a full specification of conditions that reduce the degrees of freedom of the calculation to zero.



If you are running a network client installation of Thermo-Calc and cannot enter the POLY module, this may be because all the license instances on that the license server makes available have been checked out.



Also see [POLY\\_3 Commands](#) on page 117 in the *Thermo-Calc Console Mode Command Reference*.

1. Define your system (see [Defining a System in Console Mode](#) on page 127).
2. Go to the POLY module. At the SYS prompt, type `GOTO_MODULE` and enter `POLY`.

3. Use `SET_CONDITION` followed by conditions and value assignments to set the conditions of your calculation. For example, to set temperature, pressure, initial composition and system size for a Fe-Cr-C system, you might enter the following:

```
SET_CONDITION T=1200 P=1E5 W(CR)=0.18 W(C)=0.0013 N=1
```

This sets the temperature (T) to 1200 K, the pressure to 1 bar (100,000 Pascal), the mass fraction of Cr to 18 mole percent, the mass fraction of C to 0.13 weight percent, and the total amount of material to 1 mole. The fraction of Fe in the system is calculated from the fractions of Cr and C. You have to set the fraction of all the components in your system except one.

4. Use `COMPUTE_EQUILIBRIUM` to run the calculation.
5. Use `LIST_EQUILIBRIUM` to see the results of the calculation.

## Calculating an Equilibrium with a Fixed Phase

There are many ways to calculate equilibriums in Thermo-Calc. The following is one example.

You can calculate an equilibrium that has a certain amount of a certain stable phase. Use [CHANGE\\_STATUS on page 59](#) and choose `Phase` to specify the phase and the amount of that phase (in normalized mole number) that you want to set as fixed. For example, if you want to find out at what temperature a system starts to melt, enter the following:

```
CHANGE_STATUS PHASE LIQUID=FIX 0
```

You must leave the state variable whose equilibrium value you are interested in unspecified. However, if you have already specified that state variable, you can make it unspecified again by using [SET\\_CONDITION on page 165](#) and set that state variable to `NONE`. For example, if you have given temperature a value, you can type:

```
SET_CONDITION T=NONE
```

The calculated equilibrium includes the value of the unspecified variable at which the equilibrium enters the phase that is fixed.



For an example where an equilibrium is calculated with a fixed phase, see Example 7 in [Console Mode Example Collection on page 14](#).

## Calculating an Equilibrium with Suspended or Dormant Phases

You can calculate an equilibrium under the assumption that one or several phases are `SUSPENDED` or `DORMANT` using `CHANGE_STATUS` and choose `Phase`. For example, to specify that all phases except one should be suspended, you can first suspend all phases and then enter a single phase in the following way:

```
CHANGE_STATUS PHASE *=SUSPENDED
CHANGE_STATUS PHASE FE_LIQUID=ENTERED
```



For an example where this is done, as well as where the status of phases is set to be dormant, see Example 10 in [Console Mode Example Collection on page 14](#).

---

## Property Diagrams

In this section:

---

<i>About Property Diagrams .....</i>	<i>137</i>
<i>Calculating and Plotting a Property Diagram .....</i>	<i>137</i>
<i>Calculating a Property Diagram One Phase at a Time .....</i>	<i>139</i>
<i>Calculating Several Properties in the Same Diagram .....</i>	<i>139</i>

## About Property Diagrams

When you calculate and plot a property diagram, there is only one independent state variable. Many different properties can be plotted as a function of this independent variable. For example, if the independent state variable is temperature, then the mole fractions of all phases can be plotted as a function of temperature. Or the composition of a specific phase may be plotted relative to temperature, or the activity of a component in the system as a whole or in a specific phase may be plotted relative to it.

A property diagram is plotted based on a series of equilibria that is computed while the value of one state variable is varied between a minimum and a maximum value. This variable is referred to as the stepping axis variable. In Thermo-Calc, first calculate one initial equilibrium, and then new equilibria are calculated at incremental steps in both directions on the stepping axis from the initial equilibrium. This continues until the stepping operation has covered the length of the axis between a minimum and a maximum value that is specified.



For an example of the calculation of a property diagram, see Example 8 in [Console Mode Example Collection](#) on page 14.

## Calculating and Plotting a Property Diagram

This topic explains how to calculate a property diagram in POLY. To calculate a property diagram means to calculate a series of equilibria while the value of the stepping axis variable varies between a minimum and a maximum value. With the exception of the stepping axis variable, all the state variables that you set when you calculate the initial equilibrium retain the values when the new equilibria are calculated.



[POLY\\_3 Commands](#) on page 117 in the *Console Mode Command Reference*.

### How to Calculate and Plot a Property Diagram

1. Calculate an initial equilibrium in the POLY module (see [Equilibrium Calculations](#) on page 130).
2. Use SET\_AXIS\_VARIABLE to set the axis variable, the minimum and the maximum stepping variable values and the step length. The first parameter of SET\_AXIS\_VARIABLE is the axis number. Since a property diagram only has one axis variable, this is set to 1. For example, if you want to set the axis variable to temperature, and calculate an equilibrium at every 50 K between a minimum temperature of 100 K and a maximum temperature of 2000 K, enter

```
SET_AXIS_VARIABLE 1 T 100 2000 50
```





An axis variable must be a state variable that is set when you calculated the initial equilibrium. For example, if you set the fraction of a component in number of moles, then you cannot set the mass fraction of this component as an axis variable. Also, the minimum stepping variable value must be smaller than, and the maximum value larger than, the value that you set the state variable to when calculating the initial equilibrium.

3. Use STEP\_WITH\_OPTIONS and choose `Normal` to perform the stepping operation.

Thermo-Calc lists the phase regions along the stepping axis, the phases contained in each region, and the number of equilibria calculated in that region. Each region is defined by the phases it contains.



The number of equilibria calculated is not just the number of steps that are performed according to the step length and the minimum and maximum values on the axis variable. This is because Thermo-Calc calculates extra equilibria when a new phase is discovered in order to determine the phase region boundary more precisely.

### Step with Options Example

```
POLY_3:s-a-v 1 T 1000 2000 100
POLY_3:step
Option? /NORMAL/:
No initial equilibrium, using default
Step will start from axis value    1000.00
...OK

Phase Region from    1000.00    for:
    BCC_A2
    GRAPHITE
Global check of adding phase at  1.01118E+03
Calculated      4 equilibria

Phase Region from    1011.18    for:
    BCC_A2
    FCC_A1
    GRAPHITE
Calculated      2 equilibria

Phase Region from    1011.18    for:
    FCC_A1
    GRAPHITE
Global test at  1.09000E+03 .... OK
Global check of removing phase at  1.15727E+03
Calculated      17 equilibria
```

4. To plot the diagram, use POST to open the POST module and then use PLOT\_DIAGRAM. By default, the X-axis represents the stepping axis variable and Y-axis represents the sum of the mole fractions of all phases (NP(\*)).

## Calculating a Property Diagram One Phase at a Time

There are many ways to calculate property diagrams in Thermo-Calc. One example is where you can calculate a property diagram with a separate stepping operation being performed for each phase at a time in its default most stable composition (the major constitution). This is useful if you want to create a property diagram for a heterogeneous system with both ordered phases and their disordered pairs.

To calculate a property diagram one phase at a time, use [STEP\\_WITH\\_OPTIONS](#) on page 172 and when prompted choose `One_phase_at_time` to perform the stepping operation.

## Calculating Several Properties in the Same Diagram

There are many ways to calculate property diagrams in Thermo-Calc. The following is another example. If you perform several stepping calculations after each other, the results of these calculations are all saved in your workspace file. This allows you to the following:

- Calculate (and then plot) missing parts of a specific property inside the first property diagram. These parts are calculated inside the range of the stepping variable with a different control condition.
- Calculate (and then plot) two or more sets of a specific property on the same property diagram for the same system. These can be calculated under different control conditions with stepping operations being performed across the same stepping axis variable range.
- Calculate phase boundary lines and then plot them in a corresponding phase diagram for the same system. This can be especially useful for some defined secondary phase-transformations. For example, if you want to find the phase boundary between BCC\_A1 and BCC\_B2, or the equal-Gm for two specific phases, or the equal-fraction or equal-activity for two specific phases of a certain species, then this can be useful.

Unless you have opened a new workspace file previously using `SAVE_WORKSPACES`, the results of the stepping calculations are saved in a `RESULT.POLY3` file. To save the results of several stepping calculations in a file different from the workspace file that your results are currently saved to, then use `SAVE_WORKSPACES` before you perform the first stepping calculation.



`SAVE_WORKSPACES` overwrites and deletes the results of all previous stepping calculations.

---

# Phase Diagrams

In this section:

---

<i>About Phase Diagrams .....</i>	<i>141</i>
<i>Calculating and Plotting a Phase Diagram .....</i>	<i>141</i>
<i>Calculating a Quasi-Binary Phase Diagram .....</i>	<i>142</i>
<i>Calculating a Quasi-Ternary Phase Diagram .....</i>	<i>143</i>

## About Phase Diagrams

Phase diagrams have two or more independent axis variables. Any state variable that has already been set can be used as the mapping variable for a mapping calculation and then as the axis variable for a phase diagram. From a mapping calculation, many types of phase diagrams can be plotted, with one of the mapped variables as one axis variable, and with other mapped variables or any varied property (state or derived variables) or entered symbol (variables, functions or table values) as the other axis variables.

All phase diagrams consist of zero phase fraction lines. There are two distinct types of phase diagrams: those with the tie-lines in the plane of the diagram and those where the tie-lines are not in the plane. The former includes binary phase diagrams and ternary isotherms. The latter includes more general isopleth diagrams with one or more fixed extensive variables (normally, this is a composition). The BIN and TERN modules calculate binary and ternary phase diagrams. The POTENTIAL and POURABIX modules calculate the more general isopleth diagrams and other related diagrams.

The following topics describe how to calculate the types of phase diagrams in the [POLY\\_3 Commands on page 117](#) module. In POLY, you can calculate phase diagram for systems with up to 40 components and with thousands of phases. You can combine activity conditions and fixed phase status and fraction conditions in any way. Thermo-Calc can calculate any arbitrary 2D section through composition space.



There is no guarantee that the conditions set will result in a calculation that reaches an equilibrium.



For an example of the calculation and plotting of a phase diagram, see Example 4 in [Console Mode Example Collection on page 14](#).

## Calculating and Plotting a Phase Diagram

This topic describes how to calculate a phase diagram in the POLY module. The commands are described in [POLY\\_3 Commands on page 117](#) and [POST Commands on page 188](#).

1. Calculate an initial equilibrium in the POLY module (see [Equilibrium Calculations on page 130](#)).
2. Use SET\_AXIS\_VARIABLE to set the first axis variable, its minimum and maximum mapping value and the length of each incremental step on this axis. The first parameter of SET\_AXIS\_VARIABLE is the axis number and is set to 1. For example, suppose you want the mass fraction of C as your first axis variable. You want it to vary between 0 and 0.1, with the length of each incremental step being no more than 0.002. You then enter:

```
SET_AXIS_VARIABLE 1 W(C) 0 .1 0.002
```



An axis variable must be a state variable that is set when you calculated the initial equilibrium. For example, if you set the fraction of a component in number of moles, then you cannot set the mass fraction of this component as an axis variable.

- Use SET\_AXIS\_VARIABLE to set the second axis variable and specify its minimum, maximum, and step length values. The axis number is set to 2. For example, suppose you want temperature as your second axis variable and you want it to vary between 900 K and 1900 K, with an incremental step of 25 K. You then enter:

```
SET_AXIS_VARIABLE 2 T 900 1900 25
```

- If you want more than two axis variables, then use SET\_AXIS\_VARIABLE until you have set all the axis variables. You can set up to five axis variables. Axis variables 3, 4 and 5 must be set temperature, pressure or to the chemical potentials of components.

You may want to save your workspace with SAVE\_WORKSPACES before you perform the mapping calculation. This saves the axis variables you have set. However, it overwrites the results of any previous stepping or mapping calculations done.

- Use MAP to perform the mapping calculation. The console lists the phase region boundaries and the phases contained on one side of each boundary.

```
Phase region boundary 30 at: 1.363E+03 2.012E-01
  FCC_A1
  ** GRAPHITE
Calculated. 3 equilibria
Terminating at known equilibrium

Phase region boundary 31 at: 1.990E+03 2.526E-01
  LIQUID
  ** GRAPHITE
Calculated. 13 equilibria
Terminating at known equilibrium
```

- To plot the diagram, use POST to open the POST module and then use PLOT\_DIAGRAM. By default, the X-axis represents mapping axis variable 1 and the Y-axis represents mapping axis variable 2.

## Calculating a Quasi-Binary Phase Diagram

There are many ways to calculate phase diagrams in Thermo-Calc. The following is an example where a quasi-binary phase diagram is used for calculations on a ternary system in which one component has an

activity or chemical potential that is fixed (although if you have fixed a phase and the phase composition varies, then the activity or chemical potential may also vary). The tie-lines in a quasi-binary diagram are in the diagram's plane of the diagram. This means that the calculation follows the lever rule as well as other rules.



For an example of a calculation of a quasi-binary phase diagram, see Example 17 in [Console Mode Example Collection](#) on page 14.

## How to Calculate a Quasi-Binary Phase Diagram

Use `CHANGE_STATUS` to set the component that has a fixed activity or chemical potential. For example, suppose you want to compute a phase diagram for a Ca-Fe-O system in which the liquid oxide (`FE-LIQ`) is in equilibrium with liquid Fe. You then enter:

```
CHANGE-STATUS FE-LIQ=FIX 0
```

## Calculating a Quasi-Ternary Phase Diagram

There are many ways to calculate phase diagrams in Thermo-Calc. The following is an example of a quasi-ternary phase diagram used for calculations on a quaternary system where one component has a fixed activity or fixed chemical potential.

### How to Calculate a Quasi-Ternary Phase Diagram

When calculating a quasi-ternary phase diagram it is necessary to set a condition on either activity or chemical potential of the fourth component. To specify a meaningful value it is recommended that you first change the component's reference state using `SET_REFERENCE_STATE`. For example, to calculate a phase diagram for a quasi-ternary Fe-Cr-Ni-C system with fixed carbon activity, you can enter the following:

```
SET_REFERENCE_STATE C GRAPH , ,
```

You must also use `SET_CONDITION` to set the activity of the component whose activity or chemical potential you have fixed. Do this by assigning a value to the ACR state variable. For example, if the component is carbon, you might enter

```
SET_CONDITION ACR(C)=0.002
```

---

## Scheil Simulations

In this section:

---

<i>About Scheil Simulations .....</i>	<i>145</i>
<i>Simulating a Scheil-Solidification .....</i>	<i>146</i>
<i>Plotting Additional Scheil Simulation Diagrams .....</i>	<i>148</i>

---

## About Scheil Simulations

Thermo-Calc is primarily a program for performing equilibrium calculations, but some non-equilibrium transformations or partial-equilibrium transformations can be simulated. One example of such a transformation is a Scheil-Gulliver solidification.

In a Scheil-Gulliver solidification, the diffusion in the solid phases is assumed to be so slow that it can be ignored, while the diffusion in the liquid phase is assumed to be very fast. With this approximation, the conditions at the liquid/solid interface can be described as a local equilibrium.

By making a stepping operation on the temperature variable (or enthalpy or amount liquid phase) with small decrementing steps, the new composition of the liquid can be determined. After each step, the amount of formed solid phase is removed and the overall composition is reset to the new liquid composition. In effect, the whole system is described as a non-equilibrium state regarding various parts of solidified phases at various solidification stages.

### The Scheil Module

You can simulate Scheil-Gulliver solidification processes with the SCHEIL module. When you enter the module, you are prompted to answer a series of questions about which database to use, what the major element is and in which amount. Thermo-Calc then displays a property diagram showing how the fraction of solid phase varies with temperature (in Celsius). You can then plot diagrams using other variables you are interested in. Do this by starting a new simulation, by opening an old file with the results of a previous simulation that you can plot differently. For example, you might be interested in plotting the fraction of remaining liquid against temperature, the fraction of each solid phase or the total of solid phases against temperature, the microsegregation in each solid phase, or the latent heat evolution against temperature.

It is possible to use the SCHEIL module to run a modified Scheil-Gulliver simulation that also takes back-diffusion of some fast-diffusing interstitial elements such as C or N into account, as well as BCC to FCC phase transformation phenomena.

### Scheil Module Examples

- See Examples 15 and 30 to simulate non-equilibrium transformations without considering fast-diffusion elements.
- See Example 48 to simulate partial-equilibrium transformation with fast-diffusion elements taken into consideration. This example also shows how you can perform lever-rule calculations (full-equilibrium transformations).

### Scheil and the Diffusion Module (DICTRA)



If you also have a license for the Diffusion Module (DICTRA), you can import a previously calculated Scheil segregation profile into the software using the command `INPUT_SCHEIL_PROFILE`. Search the online help or see the *Diffusion Module (DICTRA) Command*





Reference.

## Simulating a Scheil-Solidification

Simulating a Scheil-Gulliver solidification process involves calculating the liquid composition of a higher-order multicomponent system at each step of a cooling process, and resetting the liquid composition as the composition of the entire system (after having removed all amount of solid phase).



[SCHEIL Commands on page 235](#) in the *Console Mode Command Reference*.

### How to Simulate a Scheil-Solidification

1. Use `GOTO_MODULE SCHEIL` to enter the SCHEIL module.
2. Type `START-WIZARD`.
3. Specify which `Database` to use.
4. Specify the `Major element or alloy` in your system.

For example, for a steel/Fe-alloy, enter `Fe`, for an Al-based alloy, enter `Al`, and for a Ni-based super alloy, enter `Ni`.

5. Set whether to specify the `Composition input in mass (weight) percent` (the default) or in `Mole percent`. Enter `Y` for mass percent and `N` for mole percent.
6. Specify the name of the `1st alloying element`. You can directly specify mass or mole percent after the name (for example, enter `Cr 5`). If this is not specified, then you are prompted to enter it separately.
7. Specify the other alloying elements in the same way as you specify the first (for example, `c 1`).
8. After you have specified your last alloying element, press <Enter> when requested to specify the next element. This ends the process of defining the bulk composition of the alloy system.

You can also specify all the alloying elements and their corresponding compositions on the same line when you are prompted to specify your first alloying element in Step 6. For example, you can enter `Cr 5 Ni 1 Mo 0.5 C 0.01 N 0.02`.

9. Specify the starting `Temperature (C)` in Celsius. The default is 2000.

This value should be sufficiently high so that the solidification simulation starts with the alloy system in the liquid single-phase region.

- 
10. Decide which phases (if any) to reject at the `Reject phase(s)` prompt. Enter the name of the phases to reject or press `<Enter>` for `NONE`.
  11. Decide whether to `Restore phase(s)`. You may want to restore a phase that you rejected when you ran the simulation earlier, or you may want to restore a phase that is rejected by default in your database. Enter the name of the phases to restore or press `<Enter>` for `NONE`.
  12. When prompted `OK?` type `N` to go back to Step 9 to reconsider which phases to reject or restore. Type `Y` to continue.

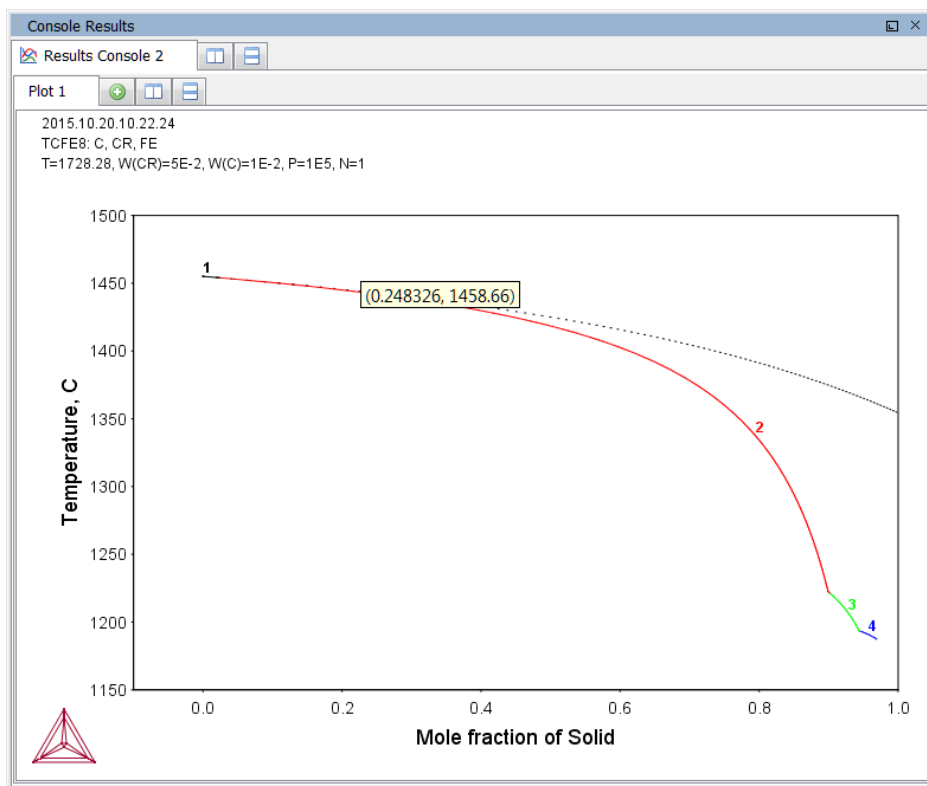
Thermodynamic data about the alloy system you defined is retrieved from the database.

13. At the `Should any phase have a miscibility gap check` prompt, press `<Enter>` for `N` or answer `Y`.

If you answer `Y`, you are prompted to specify the `Phase with miscibility gap`. Answer with a solution phase name(s) (in this example `FCC` is entered) as well as the `Major constituents for sublattice` (for each sublattice site) (for this example, `Cr` is entered for sublattice 1 and `C` for sublattice 2). In this example the `Phase with miscibility gap` is `LIQUID PHASE`  
NAME: `LIQUID`.

14. Press `<Enter>` to specify another phase.
15. Specify the names of any `Fast-diffusing components`. Press `<Enter>` for `NONE` or type all the names on the same line then press `<Enter>`. If you do specify any fast-diffusing components, then you are prompted to set whether `BCC to FCC` phase transformations should be simulated.

The Scheil-Gulliver solidification simulation runs, and the default diagram (Temperature versus Mole Fraction of Solid) is automatically plotted in the Console Results window.



## Plotting Additional Scheil Simulation Diagrams

Post processing is done the same way as POLY-3 (see [POLY\\_3 Commands](#) on page 117), specific variables for plotting in the Scheil Module are listed.

### Abbreviations for Scheil State Variables

The variables can be plotted along the X- and Y-axes. In the table, *ph* is an abbreviation of *phase*, and *el* is an abbreviation of *element*. Use the abbreviations of the variables when you specify what the X- and Y-axes represent in a diagram.

Abbreviation	State variable
T	Temperature in Celsius
NL/BL	Mole/mass fraction of liquid
NS/BS	Mole/mass fraction of all solid phases
NS(ph)/BS(ph)	Mole/mass fraction of a solid phase
W(ph,el)	Weight fraction of an element in a phase
X(ph,el)	Mole fraction of an element in a phase

---

Abbreviation	State variable
Y(ph,el)	Site fraction of an element in a phase
NN(ph,el)	Distribution of an element in a phases
NH/BH	Heat release and Latent heat per mole/gram
CP/BCP	Apparent heat capacity per mole/gram
NV/NV(ph)	Molar volume of the system or a phase
DS/DS(ph)	Average density of the system or a phase
BT	Apparent volumetric TEC of the system

---

# T0 Temperature Simulations

In this section:

---

<i>T0 Temperature Simulations .....</i>	<i>151</i>
<i>Making a T0 Temperature Simulation .....</i>	<i>151</i>

## T0 Temperature Simulations

The T0-temperature is the temperature at which two phases have the same Gibbs energy for a certain composition in a multicomponent system. The  $T_0$ -temperature is located within the two-phase field between the phases and it is the theoretical limit for a transformation without diffusion. T0-temperatures are often of interest if you want to understand how diffusionless transformations work. The T0 temperature in a multicomponent system with a fixed composition is temperature at which the tangent lines of the Gibbs energies of the two target phases are the same.

If the composition of one or two components varies, the common Gibbs energy for the two phases in partial equilibrium of a diffusionless transformation becomes a plane or surface, and the T0 temperature becomes a line or plane.



See Examples 23 and 41 in the *Console Mode Examples*.



Also see [Making a T0 Temperature Simulation](#) below for step-by-step instructions, as well as *Console Mode POST Module* on page 179.

## Making a T0 Temperature Simulation

This describes how to perform a T0 temperature simulation and apply a stepping calculation to its initial result.

Before you perform a T0 temperature calculation, you must have defined your initial system and be in POLY. The initial overall composition must have appropriate settings for the desired T0 temperature calculation for the two target phases.



See [POLY\\_3 Commands](#) on page 117 in the *Thermo-Calc Console Mode Command Reference*.

### How to Make a T0 Temperature Simulation

1. Use SET\_CONDITION to set the conditions of your calculation in the same way as when you calculate an ordinary equilibrium.
2. Use COMPUTE\_EQUILIBRIUM to run the calculation. The calculation does not need to reach an equilibrium in which any of the target phases is stable.
3. When you have calculated your initial equilibrium, use ADVANCED\_OPTIONS and choose T-zero.
4. When prompted, specify the names of the two target phases for which the T0 temperature (where the phases' Gibbs energies are equal) is to be calculated.
5. If the T0 temperature between the two target phases is calculated, this temperature (in

Kelvin) is shown in the Console window.

6. If you want to do a stepping calculation based on this initial T0 temperature calculation, then use SET\_AXIS\_VARIABLE to specify which state variable to use as the stepping variable. This is done the same way as when you calculate a normal property diagram.



When a T0 temperature simulation is run, you cannot set temperature as the stepping variable.

7. Use STEP\_WITH\_OPTIONS and choose T-zero to initiate the stepping calculation. You are prompted to specify the names of the target phases for which the T0 temperature is calculated.

During the STEP T-ZERO calculation procedure, the calculated T0 values are presented next to the stepping variable.

For example, part of the output might look like this:

```
Phase Region from 1.000000E-01 for:
BCC_A2
FCC_A1
1.000000E-01      940.24
9.250000E-02      941.20
2.500000E-03      977.61
7.500000E-09      979.34
```

When the stepping calculation has finished, you can move to the POST module and plot the T0 line against the stepping composition variable or another varying axis value. Or you can impose the calculated T0 line onto a normal phase diagram.

---

# Paraequilibrium

In this section:

---

<i>About Paraequilibrium</i> .....	154
<i>Calculating a Paraequilibrium</i> .....	154



## About Paraequilibrium

A paraequilibrium is a partial equilibrium where one interstitial component (such as carbon C and nitrogen N) in a multicomponent alloy can diffuse much faster than the other components (the substitutional elements, including the matrix element and alloying elements). The chemical potential for the interstitial component in two partially equilibrated phases is equal in such a case, but this is not true for the other components. In such a paraequilibrium state, it is possible to have a transformation that is partly without partitions, where a new phase of the mobile component can form with different content but where the slowly diffusing components retain their compositions.

A paraequilibrium calculation is useful when, for example, you want to study phase transformations in systems with large differences in the diffusivities of different elements. Transformations occurring under paraequilibrium states can be much more rapid than if full local equilibrium holds at the phase interface.



See Example 42 in the *Console Mode Examples*.



Also see [Calculating a Paraequilibrium](#) below for step-by-step instructions.

## Calculating a Paraequilibrium

This topic describes both how to calculate an initial paraequilibrium with two target phases, and how to base a stepping calculation on this initial calculation.

Before you do any paraequilibrium calculations, you must have defined your initial alloy system and be in POLY. The initial overall composition must have appropriate settings for the desired paraequilibrium calculation for the two target phases.

### How to Calculate a Paraequilibrium



These commands are described in the *Thermo-Calc Console Mode Command Reference* included with this documentation set.

1. Use SET\_CONDITION to set the conditions of your calculation just like when you calculate an ordinary equilibrium.
2. Use CHANGE\_STATUS to set the status of the chosen interstitial components to SPECIAL. For example, if C is an interstitial component, enter:

```
CHANGE_STATUS COMPONENTS C=SPECIAL
```

This gives you a clear picture on u-fractions of the substitutional and interstitial components, which are different from the overall composition in the system. The SPECIAL status means that the specified components are not included in summations for mole or mass fractions. Therefore, all the composition variables plotted from paraequilibrium calculations are u-fraction related quantities.

3. Use `COMPUTE_EQUILIBRIUM` to run the calculation.
4. When you have calculated your initial equilibrium, use `ADVANCED_OPTIONS Paraequilibrium` to perform the paraequilibrium calculation.
5. Specify the names of the target phases of the paraequilibrium state. For example, `FCC#1 BCC` and `FCC#2 M23C6`.



Both phases must have similar interstitial/vacancy sublattices that the fast-diffusion interstitial components occupy. Both target phases should have phase constitution definitions that cover all the defined substitutional and interstitial components of the current alloy system.

6. Specify the names of one or more fast-diffusing components. These components must be located on the interstitial/vacancy sublattices in both of the chosen phases.



Interstitial components (for instance C and N combined) may have significantly different behaviours depending on how they are partitioned in different structured phases.

If the paraequilibrium between the two specified phases is successfully calculated, then a message is displayed, for example:

```
NP(FCC) = 0.3586 with U-fractions C = 2.71821E-02 N = 4.1548129E-03
NP(BCC) = 0.6414 with U-fractions C = 7.10061E-04 N = 2.3781027E-04
All other compositions are the same in both phases
```

The first two lines show the phase amounts expressed in mole-percent [NP(phase)] and the contents of the interstitial components C and N in each phase. These contents are expressed in u-fractions. The third line states that the compositions of the matrix component and all the remaining compositions (regarding substitutional components) are equal in the two target phases at the paraequilibrium state.

7. If you want to do a stepping calculation based on this initial paraequilibrium, then use `SET_AXIS_VARIABLE` to specify which state variable to use as the stepping variable. This is done exactly in the same way as when you calculate a normal property diagram.
8. Use `STEP_WITH_OPTIONS → Paraequilibrium` to initiate the stepping calculation. You are prompted to specify the names of the target phases of the paraequilibrium states as well as the fast-diffusing components.

The stepping calculation is performed, and the different phase regions are listed with columns for the value of the stepping variable, the amounts of the two target phases, the u-fractions of interstitial(s) in each of the two phases, and the LNACR value(s) of the interstitial component(s).

## Example

This command calculates a paraequilibrium between two phases.  
 You must calculate an equilibrium with the overall composition first.  
 Name of first phase: fcc\_a1  
 Name of second phase: bcc\_a2  
 Fast diffusing component: /C/: C  
 Fast diffusing component: /NONE/:  
 Output during stepping is:  
 axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,  
 and LNACR value(s) of interstitial(s)

Phase Region from	900.000	for:				
BCC_A2						
FCC_A1						
9.000000E+02	0.176	0.824	4.977501E-02	6.609390E-04	-2.303643E-01	
8.900000E+02	0.161	0.839	5.421135E-02	6.889794E-04	-1.689777E-02	
8.800000E+02	0.148	0.852	5.872152E-02	7.140931E-04	1.943989E-01	
8.700000E+02	0.137	0.863	6.329608E-02	7.362105E-04	4.040959E-01	
8.600000E+02	0.127	0.873	6.792661E-02	7.552871E-04	6.126989E-01	
8.500000E+02	0.119	0.881	7.260558E-02	7.713010E-04	8.206607E-01	
8.400000E+02	0.111	0.889	7.732629E-02	7.842505E-04	1.028392E+00	
8.300000E+02	0.105	0.895	8.208278E-02	7.941530E-04	1.236267E+00	
8.200000E+02	0.099	0.901	8.686971E-02	8.010431E-04	1.444633E+00	
8.100000E+02	0.093	0.907	9.168236E-02	8.049714E-04	1.653814E+00	
8.000000E+02	0.089	0.911	9.651648E-02	8.060032E-04	1.864114E+00	



It is possible to now move to the POST module and plot some of the results of the calculation. For an example of a paraequilibrium calculation and how it can be plotted, see Example 23 in the *Console Mode Examples*.

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## Potential Diagrams

In this section:

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<i>About Potential Diagrams .....</i>	<i>158</i>
<i>Calculating a Potential Diagram .....</i>	<i>158</i>
<i>Calculating a Potential Diagram with Different Pressure .....</i>	<i>159</i>

## About Potential Diagrams

If you have a metal-oxide/sulphide-gas interaction system, you might want to calculate a so-called potential phase diagram given certain temperature and pressure. A potential diagram uses the activities of two major species in the gaseous mixture phase as mapping variables. The activities (that is, the fugacities at 1 bar) of these two species are typically set as the X- and Y-axis when the diagram is plotted. The phase relations between the gaseous mixture and various metal forms, metal-oxides, metal-sulphides, or other metal-bearing solids, are represented by different fields controlled by these two potential quantities.

This topic describes how to calculate such potential diagrams with the POTENTIAL module, and how to later modify the pressure of such a calculation in POLY. The calculation done by the POTENTIAL module always assumes a pressure of 1 bar.



[POTENTIAL\\_DIAGRAM Module on page 217](#) in the *Console Mode Command Reference*.

## Calculating a Potential Diagram

You need access to a substance or solution database that contains a gaseous mixture phase, metals (or alloys), and solids such as metal-oxides, sulphides, sulphates, carbonates, silicates, nitrides or nitrates (stoichiometric or solution phases).



[POTENTIAL\\_DIAGRAM Module on page 217](#) in the *Console Mode Command Reference*.

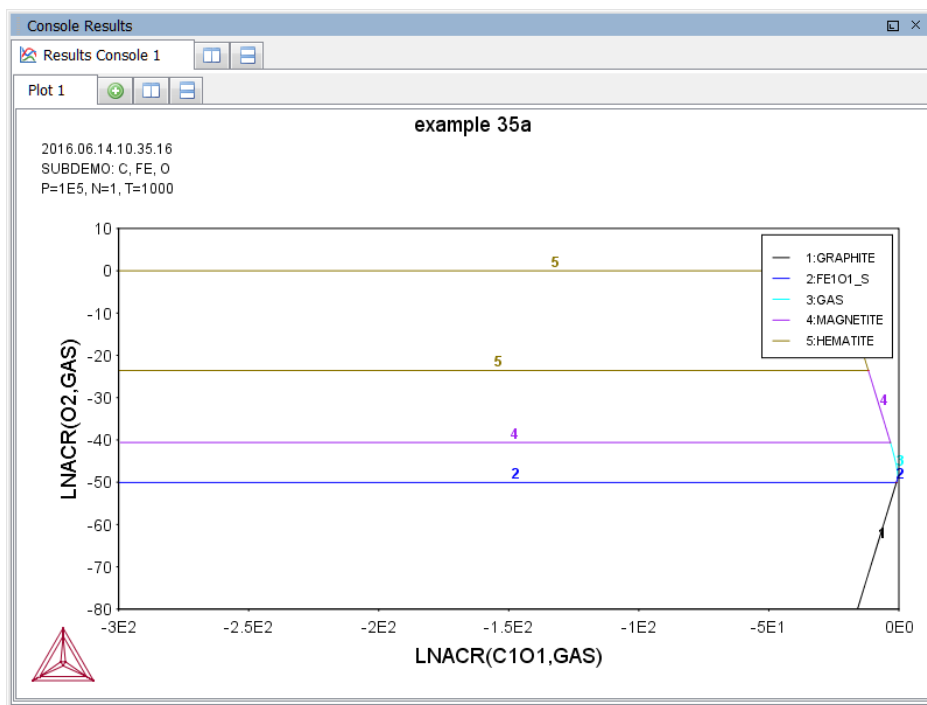
1. Use GOTO\_MODULE and enter `POTENTIAL`.
2. Specify which substance or solution database to use. Any substance or solution database can be used that has a gaseous mixture phase, metals (or alloys), and solids such as metaloxides, sulphides, sulphates, carbonates, silicates, nitrides, and nitrates (stoichiometric or solution phases).
3. Specify the matrix element (a metal) and the two gaseous species that define you metal-gas interaction system. The names of these components must be available in the database you are using.
4. Set the temperature (in Kelvin). (The pressure is always 1 bar.)

A potential diagram with the activities of the two gaseous species as mapping variables is calculated. These mapping variables are also set as the axis variables in the plotted diagram.

### Example Plot



The following is an example diagram (from example 35 in the *Console Mode Examples*).



A POLY3-file is also automatically saved in the current working directory with the default name POT.POLY3.

5. When the diagram is plotted, it opens the POST module where you can modify the plotted diagram in any way you like.

## Calculating a Potential Diagram with Different Pressure

It is possible to modify both the calculation and the plotted diagram that the POTENTIAL module generates in the POLY and POST modules. You can do this by opening a POLY3-file with the results from a POTENTIAL module calculation in either POLY or POST. You can modify the calculation in the same way that you can modify any ordinary mapping calculation or phase diagram. For example, this is useful for calculating a potential diagram at a pressure other than 1 bar.



[POLY\\_3 Commands on page 117](#) in the *Console Mode Command Reference*.

You must have calculated a potential diagram already, and have the saved POLY3-file available.

1. Use GOTO\_MODULE and enter POLY.
2. Use READ followed by the name of the POLY3-file that contains the results of the potential diagram calculation that you want to modify.

3. This opens the workspace file and loads the previous settings and results. The activities of the two gaseous species is now part of the conditions, and these conditions are set as the mapping variables.
4. Use `SET_CONDITION` to specify the pressure under which you want the potential diagram to be calculated. For example, to set the pressure to 1000 bar, enter:

```
SET_CONDITION P=1e8
```

5. Use `COMPUTE_EQUILIBRIUM` to compute the initial equilibrium.

You may also want to use `ADD_INITIAL_EQUILIBRIUM` to calculate some additional equilibria that the mapping calculations are based on.

6. Use `MAP` to perform the mapping calculations.
7. Use `GOTO_MODULE` and enter `POST` to set conditions for visualization and to plot the diagram.

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## Aqueous Solutions

In this section:

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<i>About Aqueous Solutions</i> .....	162
<i>Calculating a Pourbaix Diagram</i> .....	163
<i>Plotting Additional Aqueous Solution Diagrams</i> .....	165
<i>Stepping Calculations in an Aqueous Solution</i> .....	167
<i>Pourbaix Examples TCEX40, 40A to 40E, and TCEX53</i> .....	168



## About Aqueous Solutions

Heterogeneous equilibrium calculations involving aqueous solutions are not different from other equilibrium calculations, but the setup of the equilibrium conditions and the reference states of the system is more complex. For example, the pH and Eh values of the aqueous solution phase are normally complex functions of bulk composition, temperature and pressure conditions.

For some simple systems, thermodynamic approximations of pH-Eh calculations can be used. But Thermo-Calc also has comprehensive thermodynamic models and databases for various non-ideal solution phases. These let you accurately calculate pH and Eh property diagrams (and many other types of property diagrams) in complex aqueous solutions in a variety of conditions.

A Pourbaix diagram is a pH-Eh phase diagram where the tie-lines are not in the plane. The chemical potentials or activities of two system components ( $H^+$  and EA) are used as mapping variables and the pH and Eh quantities are normally plotted on the X- and Y-axes of the diagram. You can use many other properties as axis variables in various property diagrams for the interaction system at a specific temperature and pressure. The phase relations between the aqueous solution and various metal forms, oxides, hydroxides, sulphides, sulphates, nitrates, silicates, carbonates and other solids, or gaseous mixtures, are represented as different fields defined by acidity and electric potential.

You can calculate Pourbaix diagrams with the Pourbaix module. The compositional definition and variations and the basic solvent and electron components  $H_2O$ ,  $H+1$  and  $ZE$  are automatically determined by the aqueous solution phase in the Pourbaix module.

### Key Components

These key components are defined as follows:

Component	Component status	Reference state	Ref-T(K)	Ref-P(Pa)
$H_2O$	ENTERED	AQUEOUS	*	100000
$H+1$	ENTERED	SER		
$ZE$	ENTERED	REFERENCE_ELECTRODE	*	100000

Besides the aqueous solution phase, your system may also contain a gaseous mixture phase. Other neutral and charged gaseous species may also be constituents. For multicomponent systems there are normally also some interacting solid phases (stoichiometric or solution) as the so-called secondary phases. These are typically the matrix and/or precipitate phases in the alloys of interest.

Some databases have been specially developed for the Pourbaix module's diagram calculations. Such a database contains all necessary phases, i.e., an aqueous solution phase, a gaseous mixture phase, some alloy solid solution phases and some secondary solid phases. Databases developed for the Pourbaix module include *PAQ* (TCS Public Aqueous Solution Database) or *PAQS* (TGG Public Aqueous Solution Database).



If such a dedicated Pourbaix module is not used, then an aqueous solution database such as *TCAQ* (TC Aqueous Solution Database), *AQS* (TGG Aqueous Solution Database), or any user-specified aqueous databases can be used. This database contains at least the *AQUEOUS* and *REFERENCE\_ELECTRODE* phases. The aqueous solution database needs to be appended with additional required data and phases, such as interacting alloy (solid) solution phases and secondary (solid and liquid) phases. Additional data is from one or more databases, such as *SSUB/SSOL/TCFE* or other substances/solutions databases.

## Calculating a Pourbaix Diagram

The *POURBAIX* module lets you construct Pourbaix diagrams and other types of property diagrams for heterogeneous interaction systems with aqueous solution phases.

When calculating a Pourbaix diagram, you need to have a database with an aqueous solution phase (that is, a phase with water as the dissolving solvent and with aqueous cation/anion and complex species as the dissolved solutes). Due to restrictions of aqueous solution models (*SIT*, *HKF*, *Pitzer*) used in the Thermo-Calc software, the aqueous solution database must be designed in the same Thermo-Calc database format as that used in the *PAQ*, *PAQS*, *TCAQ* and *AQS* databases for the aqueous solution phase.

Pourbaix diagram calculations are done in the advanced Pourbaix module.



*POURBAIX\_DIAGRAM* Commands on page 219 in the *Console Mode Command Reference*.

## How to Calculate a Pourbaix Diagram

1. At the `SYS` prompt, enter `GOTO_MODULE POURBAIX`.
2. At the `Need any instruction on the POURBAIX module?` prompt, press `<Enter>` to skip or enter `Y` to learn more.
3. Press `<Enter>` at the prompt `Enforce a PAUSE after plotting when running a MACRO?`.
4. Press `<Enter>` to accept the default `1` to `Start a completely new POURBAIX diagram calculation` or enter `3` to `Open an old file and make another POURBAIX calculation`.

To choose `3`, you must have already done a Pourbaix calculation and have it saved in a *POLY3*-file. The new calculation uses the same system definition as the previous calculation, but the other conditions, such as the bulk composition, temperature and pressure, can be modified in the next step.

5. Type `Y` or `N` to set whether to `Consider the GAS phase (gaseous mixture phase) in the calculation`.

The gaseous mixture phase should at least contain H<sub>2</sub>O, O<sub>2</sub> and H<sub>2</sub>. If a GAS phase is not considered, then only the interactions between the aqueous solution phase and various solid phases (alloy phases and secondary phases) are calculated. Such a calculation may not accurately present all the heterogeneous interactions. Some secondary phases are therefore usually needed. Such phases exist in the PAQ or PAQS Public Aqueous Solution Databases. They can also be appended from the SSUB/SSOL/TCFE or other appropriate substances/solutions databases.

6. Type **Y** or **N** to set whether to Use `single database (Y)` or a multiple database (**N**).

If you choose to use a single database, at the `Combined Database: /PAQ2/` prompt specify a database that is specially developed for the Pourbaix module's diagram calculations.

If you choose to use a multiple database, then you are prompted to specify an aqueous solution database and to append any additional required data and select necessary phases, such as various interacting alloy (solid) solution phases, and secondary (solid and liquid) phases, for example.

7. Specify all your solutes and the molality of each solute when prompted to do so. This can be done in terms of elements (such as Fe, Ni, Na, Cl, C or S) or arbitrary complex species (such as NaCl, CO<sub>2</sub>, CoCl<sub>3</sub>, Fe<sub>0.93</sub>S, NaSO<sub>4</sub>-1, or H<sub>2</sub>SO<sub>4</sub>). You can enter the element/species and the molarity on one line (for an example, NaCl 2.5).



The first letter of the element abbreviation must always be upper case. Any second letters must be lower case. When you have finished your specification, press <Enter> when asked to specify `Next solute`.

The definition of your system and its initial bulk composition is now presented.

8. Type **Y** to confirm the defined system and its bulk composition.

The thermodynamic data for your system is now retrieved from the database(s) chosen.

9. Answer the questions that you are prompted regarding various parameters of your calculation. You are asked to do any of the following:

- `Rejectphase(s)` **OR** `Restore phases(s)`
- **Check for miscibility gaps on any phase** (`Should any phase have a miscibility gap check?`)
- `Enforce the Global Minimization Technique in calculations?`
- **Save all functions, variables and tables in POLY3 file?**
- `Set numerical limits on the calculation`

- Confirm defined conditions?
  - Accept the default settings for two mapping variables
8. The Pourbaix calculation starts. Answer the question `Any missing phase boundary you could possibly think of?` Type `Y` or `N` to set whether you want to add starting points to the calculation. If you suspect that the calculation has missed some phase boundaries, this may help the program to detect them.
9. Answer questions about how the diagram is plotted and how to save the results of your calculation. You are asked to do any of the following:
- Change the pH/Eh steps for smoother curves?
  - Zoom in on a specific region of the diagram
  - Change the curve-label option for the diagram
  - Add label-texts onto the Pourbaix diagram
  - Change the subtitle of the diagram
  - Change the axis-texts
  - Further refine the diagram in the POST Module
  - Print the diagram (save a Hard copy of the diagram)
  - Save the X-Y coordinates of curve on a text file
  - Modify the diagram
  - Calculate and plot another Pourbaix diagram (`Any more diagram?`)

## Plotting Additional Aqueous Solution Diagrams

When you have calculated a Pourbaix diagram, you can plot additional diagrams based on the results of the same calculation, but with different axis variables than Ph and Eh.

The variables can be plotted along the X- and Y-axes. Use the abbreviations of the variables when you specify what the X- and Y-axes represent in a diagram. In the table, *AQsp* refers to the name of a specific aqueous species. The asterisk (\*) can be used as a wild card character for all such species. If neither *AQsp* nor \* is entered in parenthesis, then all species are searched.

You must have plotted a Pourbaix diagram to plot a diagram with other variables than Ph and Eh on the Y-axis and the X-axis. You can either plot such additional diagrams directly after having finished the plotting and saving/printing of a Pourbaix Ph-Eh diagram or by choosing option 2 (Open an old file and plot other property diagrams) when you enter the POURBAIX module and opening a POLY3 workspace file.

### Abbreviations for Aqueous Solution Variables

Abbreviation	Variable
pH	Acidity
Eh	Electronic Potential (V)
Ah	Electronic Affinity (kJ)
Pe	Electronic Activity (log10ACRe)
IS	Ionic Strength
TM	Total Concentration
Aw	Activity of Water
Oc	Osmotic Coefficient
MF(AQsp)	Mole Fractions of Aqueous Species
ML(AQsp)	Molalities of Aqueous Species
AI(AQsp)	Activities of Aqueous Species
RC(AQsp)	Activity Coefficients of Aqueous Species

### How to Plot an Aqueous Solution Diagram

1. Type **Y** when prompted whether to plot any more diagrams, or select option 2 when you enter the POURBAIX module.
2. Specify which variable you want the X-axis to represent. Use the abbreviation specified in the preceding table. When you specify the name of an aqueous species, you can use the asterisk (\*) to select all species.
3. Specify which variable you want the Y-axis to represent. The diagram is then automatically plotted.
4. Answer questions about how the diagram is plotted and how to save it. You are asked to do any of the following:
  - change the axis-type (linear, logarithmic or inverse) on the X-axis or Y-axis
  - zoom in on a specific region of the diagram
  - change the curve-label option for the diagram
  - add label-texts onto the Pourbaix diagram
  - change the subtitle of the diagram
  - change the axis-texts

- refine the diagram in the POST Module
- print the diagram (save a hard copy)
- save the X-Y coordinates of curve on a text file
- modify the plotted diagram
- calculate and plot another aqueous solution diagram

## Stepping Calculations in an Aqueous Solution



Performing the stepping calculation overwrites all the previous settings and stepping results on the POLY3-file. To avoid this, use [SAVE\\_WORKSPACE](#) on page 232 to create a new workspace.

When you have calculated a Pourbaix diagram, you can use the saved results of the calculation (the POLY3-file), and make a property diagram based on stepping calculation.

Since the program normally sets the calculated initial equilibrium point as the starting point, the minimum value for the stepping variable must be specified as smaller or equal to the specific initial condition, and the maximum value as larger or equal to that condition. If pH is set as the stepping variable, the program automatically calculates the equilibrium constant in logarithmic ( $\log_{10}K_a$ ) of the electrolysis reaction  $\text{H}_2\text{O (water)} = \text{H}^+ + \text{OH}^-$  for the real aqueous solution under the current temperature-pressure-composition conditions, and thus this constant  $\log_{10}K_a$  value is considered as the highest pH in specifying the maximum value along stepping. Subsequently, confirm or modify an increment factor with a default value; for pressure and mole of a component, specify the step in logarithmic ( $\log_{10}P$  or  $\log_{10}N$ ).

### State Variable Abbreviations

You can use any of these state variables as a stepping variable.

State variable	Abbreviation
Temperature (K)	T
Pressure (bar)	P
Acidity	pH
Electronic potential (V)	Eh
Mole number of a dissolving component (such as Fe, Na, Cl, or NaCl) in 1 kg of water.	N(Comp) (for example, N (Fe) )

### How to Do a Stepping Calculation

You must have plotted a Pourbaix diagram before making a stepping calculation on an aqueous solution.

1. Use GOTO\_MODULE POURBAIX to enter the POURBAIX module.
2. Type 4 to Open an old file and make another STEPPING calculation.
3. Choose which POLY3-file to load.
4. Specify the conditions of the calculation by answering the questions that follows.

The system definition is the same as in the previous Pourbaix calculation, but you can modify conditions such as bulk composition, temperature and pressure, and change some component definitions if necessary.

5. Specify which variable to use as the stepping variable (see the preceding table), its minimum and maximum value, and the length of each incremental step.

The settings and stepping results are written to the opened POLY3-file, and a first default property diagram is plotted.

## Pourbaix Examples TCEX40, 40A to 40E, and TCEX53

### NOTES about TCEX40A and TCEX40E

In order to be able to subsequently run the TCEX40B (Main Option 2), TCEX40C (Main Option 3) and TCEX40D (Main Option 4), which open the previously-saved POURBAIX-type calculation POLY3 file, the user should make four copies of the resulting POURBAIX.POLY3 as TCEX40A.POLY3, TCEX40B.POLY3, TCEX40C.POLY3 and TCEX40D.POLY3.

However, this has to be properly done outside of the TCCS software after the TCEX40A is executed. The reason is that, if saving the POLY3 workspace of the POURBAIX calculation results in the POLY3-module monitor (through the command sequence "GO PLOY3" and "SAVE TCEX40A.POLY3 Y"), all the initial equilibrium points and the mapping/stepping calculation results will be lost, and parts of the POLY3 file structure (e.g., some definitions of the previously defined POURBAIX-type calculation system) will be destroyed. In principle, before executing any Main Option (for calculations and graphical processing), it is highly recommended that the user shall save/rename/copy the previously-generated POLY3 file as another POLY3 file. Only in this way, it can avoid destroying the previous-saved POURBAIX-type calculation results.

Under Windows DOS-session (outside TCCS):

- copy POURBAIX.POLY3 TCEX40A.POLY3 (or TCEX40E.POLY3)
- copy POURBAIX.POLY3 TCEX40B.POLY3
- copy POURBAIX.POLY3 TCEX40C.POLY3
- copy POURBAIX.POLY3 TCEX40D.POLY3

or inside TCCS (under Windows NT/2000/XP, but not Windows 95/98/ME):

- @copy POURBAIX.POLY3 TCEX40A.POLY3 (or TCEX40E.POLY3)
- @copy POURBAIX.POLY3 TCEX40B.POLY3
- @copy POURBAIX.POLY3 TCEX40C.POLY3
- @copy POURBAIX.POLY3 TCEX40D.POLY3

Under Linux/UNIX platforms (outside TCCS):

- cp POURBAIX.poly3 TCEX40A.poly3 (or TCEX40E.poly3)
- cp POURBAIX.poly3 TCEX40B.poly3
- cp POURBAIX.poly3 TCEX40C.poly3
- cp POURBAIX.poly3 TCEX40D.poly3

### Example TCEX40

- Using PAQ2 or PAQS2 database;
- For the Fe-H<sub>2</sub>O-NaCl heterogeneous interaction systems
- With the Main Option 1
- Using the Single-Database Option, i.e., retrieving data from the PAQ2 [TCS Public Aqueous Solution (SIT) Database, v2.4; using the SIT aqueous solution model] or PAQS2 [TCS Public Aqueous Solution Database, v2.4; using the Complete Revised HKF aqueous solution model]; both of which contain an AQUEOUS solution phase and REF\_ELECTRODE phase (as a reference for electron in aqueous electrolyte systems), as well as some data for various solid phases (solution or stoichiometric) and gaseous mixture phase. The PAQ2 and PAQS2 are specially designed for demonstrations of calculations of the so-called Pourbaix diagrams (i.e., pH-Eh plots) and other types of phase diagrams or property diagrams in some aqueous-bearing multicomponent heterogeneous interaction systems within the limited chemical framework of Fe-Co-Cr-Ni-C-N-S-H<sub>2</sub>O-NaCl, via the Single-Database Option in the advanced POURBAIX module or through the normal TDB-GES-PLOY-POST routine.

To further run the following Main Options:

- Main Option 2 for plotting many other property diagrams of the calculated interaction system;
- Main Option 3 for making another POURBAIX calculation of the same chemical system but under a different P-T-X condition;
- Main Option 4 for making a POLY3 STEPPING calculation of the same chemical system but varied with only one independent variable;



\*\* The Main Options 2, 3 and 4 are not illustrated in this TCEX40 example.

Five more examples (TCEX40A, TCEX40B, TCEX40C, TCEX40D and TCEX40E) are also provided to demonstrate various options and features in the POURBAIX module and to show more advanced applications of the TCAQ2 and AQS2 aqueous solution databases [in the Multiple-Database Option, i.e., with appended data from the SSOL5 and SSUB5 databases].

### Example TCEX40A

- Option 1
- Using the Single-Database Option, i.e., retrieving data from the PAQ2 [TCS Public Aqueous Solution (SIT) Database, v2.4; using the SIT aqueous solution model] or PAQS2 [TCS Public Aqueous Solution Database, v2.4; using the Complete Revised HKF aqueous solution model]; both of which contain an AQUEOUS solution phase and REF\_ELECTRODE phase (as a reference for electron in aqueous electrolyte systems), as well as some data for various solid phases (solution or stoichiometric) and gaseous mixture phase. The PAQ2 and PAQS2 are specially designed for calculations of the so-called Pourbaix diagrams (i.e., Eh-pH plots) and other types of diagrams in aqueous-bearing multicomponent heterogeneous interaction systems, via the Single-Database Option in the POURBAIX module or through the normal TDB-GES-PLOY-POST routine.
- A POLY3 file called POURBAIX.POLY3 is automatically saved.
- For the purposes of recalling this file in other Main Options (as in the TCEX40B, TCEX40C & TCEX40D), the POURBAIX.POLY3 has to be renamed or copied as another file name (in this particular example, as TCEX40A.POLY3, and TCEX40B.POLY3, TCEX40C.POLY3 & TCEX40D.POLY3). Note that the renaming or copying has to be done outside TCCS, otherwise the POLY3 file structure will be destroyed. However, under WindowsNT/2000/XP environments, one can use MS-DOS commands to do so, e.g., @copy POURBAIX.POLY3 TCEX40B.POLY3
- The Main Option 1 also provides the opportunity to plot many property diagrams along phase boundaries, after the default Pourbaix diagram is generated and refined (not necessarily going through the Main Option 2).

### Example TCEX40B

- Demonstration of the Main Option 2 Graphical Processing (by plotting more diagrams); various options for refining a plotted diagram (including direct interactions with the POST Module); Graphical processing of related property diagrams.
- Reading a previously saved POURBAIX.POLY3 file (or renamed as another name, for instance, the TCEX40B.POLY3), and then plotting some property diagrams for the previously calculated system.

- The loaded POLY3 file will not be modified by this Main Option. It is thus not necessary to save the file in another name; however, it is still recommended that the user to copy the TCEX40A.POLY3 (or TCEX40E.POLY3) as TCEX40B.POLY3 before the Main Option 2 is executed in this particular example.

### Example TCEX40C

- Demonstration of the Main Option 3 Calculation (by modifying T-P-X conditions); graphical processing of a Pourbaix diagram.
- Reading a previously saved POURBAIX.POLY3 file (or renamed as another name, for instance, the TCEX40C.POLY3), and then making another POURBAIX-type calculation and graphical processing of a new Pourbaix diagram for the same chemical system but under a different P-T-X condition.
- The loaded POLY3 file will be rewritten according to the T-P-X settings in the new POURBAIX-type calculation. It is thus recommended to save the file in a new name outside of TCCS before this Main Option is proceeded (in this particular example, the TCEX40A.POLY3 is copied to TCEX40C.POLY3).
- The Main Option 3 also provides the opportunity to plot many property diagrams along phase boundaries, after the default Pourbaix diagram is generated and refined (not necessarily going through the Main Option 2).

### Example TCEX40D

- Demonstration of the Main Option 4 Calculation (by utilizing various stepping variables); graphical processing of related property diagrams.
- Reading a previously saved POURBAIX.POLY3 file (or renamed as another name, for instance, the TCEX40D.POLY3), and then making some normal POLY3 STEPPING CALCULATIONS.
- The loaded POLY3 file will be rewritten according to the T-P-X and stepping variable settings in the stepping calculation. It is thus recommended to save the file in a new file name outside of TCCS before this Main Option is proceeded (in this particular example, the TCEX40A.POLY3 is copied to TCEX40D.POLY3).
- The resulting POLY3 file (in this example, TCEX40D.POLY3) can be subsequently called by a Main Option 2 for plotting more property diagrams, or by another Main Option 4 for making other stepping calculations.
- The Main Option 4 also provides the opportunity to plot many property diagrams after the default Pourbaix diagram is generated and refined (not necessarily going through the Main Option 2).

- Exploration of the possibility of modifying the definitions for some desired system-components, through the direct and internal POURBAIX-POLY3 intersection, for a STEPPING (and/or MAPPING) calculation inside the POURBAIX Module.

### Example TCEX40E

- Demonstration of the Main Option 1 Calculation with the Multiple-Database Option; graphical processing of a Pourbaix diagram.

For a more complex application than in Example 40A.

This example requires licenses to three types of commercial Thermo-Calc databases otherwise it cannot be run, i.e.,

- A: TCAQ2 (TCS Aqueous Solution Database, v2.5; SIT model) or AQS2 (TGG Aqueous Solution Database, v2.5; HKF model);
  - B: SSUB4 (SGTE Pure Substances Database, v4) or TCMP2 (TCS Materials Processing Database, v2);
  - C: SSOL4 (SGTE Alloy Solutions Database, v4) or TCFE6 (TCS Steels/Fe-Alloys Database, v6) or ALIKE.
- This particular example uses the multiple-database combination of TCAQ2+SSUB4+SSOL4; among them, TCAQ2 database contains only an AQUEOUS solution phase (using the SIT model) and REF\_ELECTRODE phase (as a reference state for electron in aqueous electrolyte systems), SSUB4 database is appended for the Gaseous mixture phase and some pure solid phases (so-called secondary phases formed during aqueous-involving interaction processes), and SSOL database is also appended for various solid solution phases.
  - A POLY3 file called POURBAIX.POLY3 is automatically saved. By reading this POURBAIX.POLY3 file (or renamed as another name), one can further run the following Main Options: Main Option 2 for plotting many other property diagrams of the calculated interaction system; Main Option 3 for making another POURBAIX calculation of the same chemical system but under a different P-T-X condition; Main Option 4 for making a POLY3 STEPPING calculation of the same chemical system but varied with only one independent variable; The Main Options 2, 3 and 4 are illustrated in the TCEX40B, TCEX40C and TCEX40D examples.
  - For the purposes of recalling this file in other Main Options (as in the TCEX40B, TCEX40C & TCEX40D), the POURBAIX.POLY3 has to be renamed or copied as another file name (in this particular example, as TCEX40A.POLY3, and TCEX40B.POLY3, TCEX40C.POLY3 & TCEX40D.POLY3). Note that the renaming or copying has to be done outside TCCS, otherwise the POLY3 file structure will be destroyed. However, under Windows environments,

one can use MS-DOS commands to do so, e.g., @copy POURBAIX.POLY3 TCEX40B.POLY3

- The Main Option 1 also provides the opportunity to plot many property diagrams along phase boundaries, after the default Pourbaix diagram is generated and refined (not necessarily going through the Main Option 2).
- The POURBAIX module inside the TCCS software also accepts the AQS2 aqueous solution database (using the complete Revised HKF model) in the Multiple-Database Option, in addition to the TCAQ2 aqueous solution database (using the SIT model).

### Example TCEX53

- Using PAQ2 or PAQS2 database; for the Fe-X-H<sub>2</sub>O-NaCl heterogeneous interaction systems (X = Cr-Ni-Co)

Note: The PAQ2 (TCS Public Aqueous Solution (SIT) Database, v2.4; using the SIT aqueous solution model) or PAQS2 (TCS Public Aqueous Solution Database, v2.4; using the Complete Revised HKF aqueous solution model) contains an AQUEOUS solution phase and REF\_ELECTRODE phase (as a reference for electron in aqueous electrolyte systems), as well as some data for various solid phases (solution or stoichiometric) and gaseous mixture phase. Therefore, it can be used, via the Single-Database Option in the POURBAIX module or through the normal TDB-GES-PLOY-POST routine, for calculations of the so-called Pourbaix diagrams (i.e., pH-Eh plots) and other types of diagrams in aqueous-bearing multicomponent heterogeneous interaction systems.

Note: The initial bulk composition of Fe-based alloy in this demonstrating calculation is just preliminarily assigned, in which the BCC\_A2 and/or FCC\_A1 solution phase(s) are considered as of primarily interest. For practical calculations, one shall have more precise inputs for the initial bulk compositions of alloys.

---

## Console Mode TAB Module

In this section:

---

<i>Tabulation of Chemical Substances, Phases or Reactions .....</i>	<i>175</i>
<i>Tabulating a Reaction .....</i>	<i>176</i>
<i>Tabulating a Substance or Solution Phase at Fixed Composition .....</i>	<i>177</i>

---

## Tabulation of Chemical Substances, Phases or Reactions

The TAB module can be used to tabulate thermodynamic functions of any type of substance, stoichiometric phase or solution phase, or reaction. The module can tabulate thermodynamic functions of pure stoichiometric phases or solution phases at fixed composition, as well as various kinds of partial derivatives for a pure stoichiometric phase or solution phase at a given composition.

The TAB module begins by evaluating the most stable species of a substance in either a homogeneous state or in a reaction. Results are presented in a table or plotted as a graph.



Also see [Tabulating a Reaction on the next page](#).

A reaction tabulation presents you with the following properties, on rows representing different temperature levels:

- Heat capacity change /  $\Delta C_p$  (Joule/K) in column 2.
- Enthalpy change /  $\Delta H$  (Joule) in column 3.
- Entropy change /  $\Delta S$  (Joule/K) in column 4.
- Gibbs energy change /  $\Delta G$  (Joule) in column 5.

In the case of a tabulation of a substance or solution phase at a fixed composition, the properties presented are the heat capacity, enthalpy, entropy and Gibbs energy, rather than the degree of change in those properties.



Also see [Tabulating a Substance or Solution Phase at Fixed Composition on page 177](#).

You can add a 6th column to the table that shows the values of a property or user-defined function of your choice.

### Reaction Tabulation Example

```

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

```

## Tabulating a Reaction

A tabulation of a given chemical reaction provides you with data about the rate of change of the standard tabulation properties at various levels of temperature. You can also add a column for a property of your choice to the table.



[TABULATION\\_REACTION Commands on page 245 in the Console Mode Command Reference.](#)

### How to Tabulate a Reaction

1. Use GOTO\_MODULE TAB to enter the TAB module.
2. If you want to add one thermodynamic functions to the tabulation calculation, which is present in a sixth column in the table, use ENTER\_FUNCTION.

You are prompted to enter the name of the column that is given at its head, and the function itself. The following state variables can be used to define the function: G, H, S, T, P, V and H298.

3. Use `TABULATE_REACTION` followed by a formula that specifies of the reacting species and products to perform the tabulation calculation. The name of the elements must be entered in upper case letters only. Terminate the chemical reaction with a semi-colon. For example, you can enter:

```
TABULATE_REACTION 3H2+N2=2N1H3;
```

Elements that are designated with a single letter must be followed by a stoichiometry factor, even if this factor is 1. `CO` hence be interpreted as Cobalt rather than as carbon monoxide. Carbon monoxide is entered as `C1O1` or `O1C1`.

4. Set the pressure, the range of temperature that you want the tabulation to cover, and change in temperature between each row in the table. You can also specify if you want to output the calculation results to an EXP-file and whether you want any graphical output, and if so, which column you want to be plotted against temperature.

The tabulation calculation is performed and you are given a table that shows the various properties at each temperature level within the range defined.

If you have chosen to receive graphical output, then the Console Results window presents a graph that plots the column of you chose (on the Y-axis) against temperature (on the X-axis). When this graph is plotted, you are now in the POST module, where you can modify the graph in various ways.

## Tabulating a Substance or Solution Phase at Fixed Composition

A tabulation of a substance or solution phase at fixed composition provides you with data about the standard tabulation properties at various levels of temperature for a given chemical reaction. You can also add one extra property column of your choice to the table.



*[TABULATION\\_REACTION Commands on page 245](#) in the *Console Mode Command Reference*.*

### How to Tabulate a Substance or Solution Phase at Fixed Composition

1. Use `GOTO_MODULE TAB` to enter the TAB module.
2. Use `SWITCH_DATABASE` to switch to a database that contains solution-based data, such as TCFE for example.



You cannot use the default SSUB database when tabulating substances or solution phases at a fixed composition.

3. If you want to add one thermodynamic function to the tabulation calculation, which is



present in a sixth column in the table, use ENTER\_FUNCTION.

You are prompted to specify the column header and the function itself. The following state variables can be used to define the function: G, H, S, T, P, V and H298.

4. Use TABULATE\_SUBSTANCE followed by the name of the substance or solution phase to perform the tabulation calculation.
5. Set the pressure, the range of temperature that you want the tabulation to cover, and change in temperature between each row in the table. You can also specify if you want to output the calculation results to an EXP-file and whether you want any graphical output, and if so, which column you want to be plotted against temperature.

The tabulation calculation is performed and a table shows the various properties at each temperature level within the defined range.

If you have chosen to receive graphical output, then the Console Results window presents a graph that plots the column you chose (on the Y-axis) against temperature (on the X-axis). ). When this graph is plotted, you end up in the POST module, where you can modify the graph in other ways.

---

## Console Mode POST Module

In this section:

---

<i>Console Mode Visualization</i> .....	<a href="#">180</a>
<i>Plotting Diagrams</i> .....	<a href="#">180</a>
<i>Modifying Diagrams</i> .....	<a href="#">181</a>
<i>Saving Diagrams</i> .....	<a href="#">183</a>
<i>Loading Saved Diagrams</i> .....	<a href="#">183</a>

## Console Mode Visualization

The results of a calculation in Thermo-Calc can be plotted by the post-processor module, also called the POST module. The diagram is presented in the Console Results window.

In the POST module, you can define and plot various kinds of diagrams based on a calculation. You can modify diagram type, which variables to plot on each axis and between which minimum and maximum values, append experimental data from an EXP-file, change labels and symbols in the diagram, zoom in on (and out from) a certain region in a diagram, etc.

If you calculate a property or phase diagram in POLY, then you have to open the POST module yourself. If your calculation was performed by a response-driven module such as SCHEIL or POURBAIX, then the plotting of a diagram based your calculation is part of the dialogue of questions and answers you have in that module (but under the hood, the response-driven module is actually utilizing the POST module to get the plotting done).

## Plotting Diagrams

Plotting a diagram is to graphically represent how several variables (typically two variables) co-vary. Each axis in a property diagram or a phase diagram represents the value of one variable. The default variables represented by the X- and Y-axes are the following:

- If you plot a diagram based on the results of a mapping operation (a phase diagram), then by default the X- and Y-axes represent the mapping axis variables 1 and 2 (set using [SET\\_AXIS\\_VARIABLE](#) on page 164 in POLY).
- If you plot a diagram based on the results of a stepping operation (a property diagram), then by default, the X-axis represents the stepping variable (set using [SET\\_AXIS\\_VARIABLE](#)) and the Y-axis represents the sum of the mole fractions of all phases (that is, NP(\*)).



[POLY\\_3 Commands](#) on page 117 in the *Console Mode Command Reference*.

## How to Plot a Diagram

To plot a diagram, you must have already made a stepping or mapping operation in POLY (or in some cases, made a calculation as part of some opening a response-driven module), and you must have entered the POST module.

The POST command is available inside POLY. Use POST to enter the POST module

1. If you want to directly plot your diagram with the default variables represented by the X- and Y-axes, type `Plot` and press `<Enter>`. This plots a property or phase diagram with the default variables represented at each axis. If you do not want to plot your diagram with these default variables, go to the next step.

2. Use `SET_DIAGRAM_AXIS` to set which variables to plot on the X-axis and the Y-axis. For example, if you want to plot a phase diagram with pressure on the Y-axis and temperature on the X-axis, type:

```
SET_DIAGRAM_AXIS X T
SET_DIAGRAM_AXIS Y P
```

3. Use `PLOT_DIAGRAM` to plot your diagram.

## Modifying Diagrams

Modifying a diagram amounts to changing the settings that determine how the POST module presents the calculated results and plots a new diagram. Suppose that you have already plotted a binary phase diagram with the mapping axis variables temperature and mole fraction of one of your components (the Fe component, say) on the X- and Y-axes. If you then want to modify your diagram so that the Y-axis instead represents, say, the mass fraction of Fe rather than the mole fraction, then you use [SET\\_DIAGRAM\\_AXIS on page 206](#) to set diagram axis Y to `w (Fe)`, and then use [PLOT\\_DIAGRAM on page 200](#).

There are many ways in which you can modify your diagram and how it is presented. Any modification made in the plot settings is taken into account the next time you use `PLOT`.

### Modification Examples



The following commands are described in the *Thermo-Calc Console Mode Command Reference*.

The following are some of the modifications you can make.

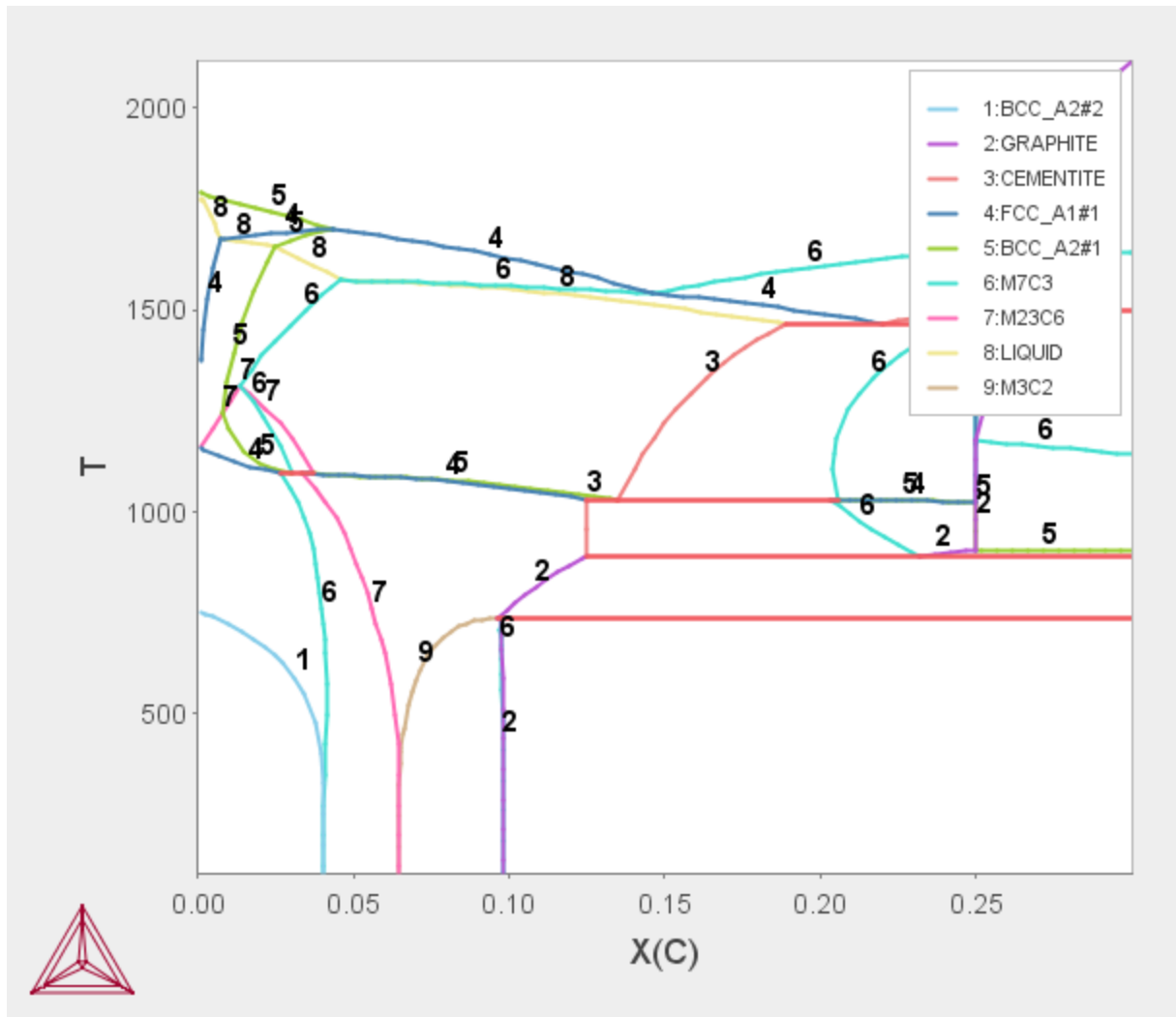
- Use [SET\\_TITLE on page 215](#) to set add a title or to change an already existing title. The title is displayed above the plotted diagram in the Console Results window.
- Use [ADD\\_LABEL\\_TEXT on page 190](#) to add a label text that starts at a certain X- and Y-coordinate. If you have plotted a phase diagram, then you can let Thermo-Calc set the label text that specifies the names of the stable phases at that coordinate.
- Use [SET\\_AXIS\\_TYPE on page 204](#) to set whether the scale of an axis is linear, logarithmic or inverse.
- Use [SET\\_DIAGRAM\\_TYPE on page 208](#) to plot a triangular diagram with the X-axis on the triangle's base and the Y-axis on the triangle's left side. Such a diagram is often useful if you want to plot the fractions of two components in a ternary diagram.
- Use [SET\\_SCALING\\_STATUS on page 214](#) to modify the range of values that are displayed on an axis. In effect, you can use it to zoom in or out of the diagram. For example, to set the scale of the X-axis to range from 0 to 0.3, type:

```
SET_SCALING_STATUS X N 0 0.3
```

The  $\times$  specifies which axis to change the scaling on, the  $N$  turns off Thermo-Calc's automatic scaling, and 0 and 0.3 specifies the minimum and maximum values on the scale. You can turn on automatic scaling again by setting the second parameter to  $Y$ .

### SET\_LABEL\_CURVE\_OPTION Example

Use *SET\_LABEL\_CURVE\_OPTION* on page 209 to label each set of curves that have the same stable phases with a certain digit. A legend is also added, where you specify which phases each digit designates.



### LTEXT vs LaTeX Commands for Labels



As of Thermo-Calc 2015a the LTEXT text formatting is replaced by LaTeX. For existing users who may have plots and files that use the LTEXT format, and especially when using Console Mode, the following examples show the command changes from LTEXT and its LaTeX equivalent:

Symbol or text format	LTEXT	LaTeX
Subscripts in an axis text	S-A-TEXT Y N Mole-fraction Al <sup>DO2</sup> O <sup>DO3</sup>	S-A-TEXT Y N \latex Mole-fraction Al <sub>2O_3</sub>
Label with subscript	add .13 .15 n c-ZrO <sup>DO2</sup>	add .13 .15 n \latex c-ZrO <sub>2</sub>
Greek symbol	ADD .05 .50 N <sup>GRd</sup>	ADD .05 .50 N \latex \delta



Also see [Changing Global Settings on page 187](#).

## Saving Diagrams

When a diagram is plotted, there are several ways in which you can save it:

- Use [DUMP\\_DIAGRAM on page 194](#) to save the diagram image to a PS, PDF, SVG, EMF, GIF, or PNG file. You are asked what format to save it in.
- To save the diagram image in a variety of image file formats, right click the diagram and select **Save Plot**.
- Use [PRINT\\_DIAGRAM on page 201](#) to print a hard copy of the diagram.



Information about the underlying calculations that the diagram is based on is not saved in an EXP-file.



Also see the *DATAPLOT User Guide* included with this documentation set.

## Loading Saved Diagrams

If you have previously saved a diagram in an EXP-file, then you can load and superimpose the diagram on another diagram. Both the following command requires you to specify which prologue and dataset(s) that are loaded from an experimental data file.

Use [APPEND\\_EXPERIMENTAL\\_DATA on page 192](#) to plot selected data from an experimental data file (EXP-file). If you have set the axes of the diagram already, the labels on the diagram are not changed when you plot the additional data from the EXP-file, irrespectively of the data in that file.

Use [QUICK\\_EXPERIMENTAL\\_PLOT on page 201](#) to plot selected data from an experimental data file (EXP-file). If you have set the axes of the diagram already, these settings are overwritten with the axes settings from the EXP-file.

## About the Database Files

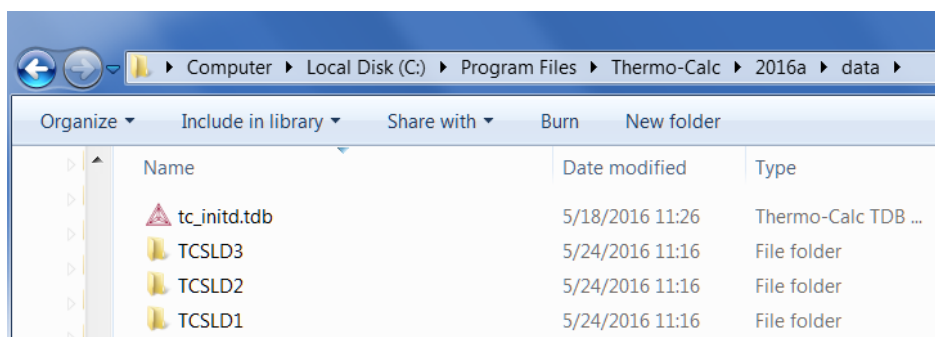
### *Encrypted vs Unencrypted Database Files*

Any licensed databases purchased from Thermo-Calc Software are encrypted in files with the extension `.TDC`; these files cannot be edited. These are referred to as *encrypted databases*.

*Unencrypted databases* have the file extension `.TDB` and can be edited. For example, PURE5 or PG35 (the free databases) or a user-defined database file. If you plan to edit any of these files, see [Editing the Database Initialization File or Unencrypted Database File on the next page](#) for information.

### *Database Installation Folder*

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



### *Database Initialization File*

In Windows, the *database initialization file* is called `tc_initd.tdb`. In Linux and Mac it is called `initd.tdb`. The file contains a list of all the databases available from Thermo-Calc Software. Individual licenses are still required to use each database.

The file is used differently by the program depending on whether you are working with databases in Console Mode or Graphical Mode. For this reason, editing the file can be problematic if you don't understand the differences. See [About Cached Database Files \(Graphical Mode only\) on the next page](#) and [Editing the Database Initialization File or Unencrypted Database File on the next page](#) for more information.

### *User Database Files*

A user-defined database is considered to be an unencrypted database because you can make changes to it.

In Graphical Mode you can add user databases via the **Options → Graphical Mode → System definer** window. Once you have added the user database it is available from the database list in the System Definer Configuration window. See [Global Settings: System Definition \(System Definer\)](#) on page 191 to add a user database.

In Console Mode, users may decide to add their own user-defined database to the database initiation file, which then makes it available in the Console window. If you plan to edit this file, see [Editing the Database Initialization File or Unencrypted Database File](#) below for important information.

## About Cached Database Files (Graphical Mode only)



Also see Global Settings [General](#) on page 188 where you can set the default database directory path.

The first time you open a database in Graphical Mode it can take a little while for it to load, especially if it is one of the large databases such as TCFE or TCNI. However, the next time the database opens quickly because now the databases are cached, or stored, in Graphical Mode.

Think of a cache as an intermediate storage area. Once a database cache is established the file made easily accessible, even if you close the software program. It is the same concept as when you load a web page for the first time. The next time the page opens faster. This is also how it works for the databases in Thermo-Calc Graphical Mode.

Thermo-Calc caches the database files, both encrypted and unencrypted types, at two points –when you first open a database, sometimes called an *in-memory cache*, and then later as a *disk-based cache*. The disk-based cache is what speeds up database loading and it is at this point that Thermo-Calc refers to the database initialization file for information. The disk-based cache uses a lookup key to find the abbreviated database name (e.g. TCFE8 or TCNI8) contained in this initialization file.



It is important to understand the way databases are cached in Graphical Mode to ensure best practices for those who also use Console Mode, especially if the database initialization file is edited. If you plan to edit this file, see [Editing a Database Initialization File or Unencrypted Database File](#) for important information.

## Editing the Database Initialization File or Unencrypted Database File

Some advanced users may decide to edit the database initialization file, for example to reorder the list of encrypted databases displaying in the Console window or to add their own user-defined database for use in Console Mode. It is important to understand that changes to this file impact the database caching process used in Graphical Mode (see [About Cached Database Files \(Graphical Mode only\)](#) above).

The following recommendations are also applicable if you edit an unencrypted database file, which includes user databases and free databases such as PURE5 or PG35.



---

## Best Practice Recommendations

If you edit the database initialization file (tc.initd.tdb in Windows or initd.tdb in Mac and Linux), then:

- If a user database is added to the file, it is subject to the same caching as the encrypted databases. This means that further changes (to the user database) will not be detected when you are working with databases in the System Definer in Graphical Mode.

If you have a user database, which is subject to regular updates, then:

- If you make changes to a user database, you then need to clear the cache.
- It is recommended that you create a separate directory to store unencrypted database files.

If you edit an unencrypted database file included with the installation (such as the PURE5 and PG35 files):

- Do not edit the file in the installation folder. Instead make a local copy and load it into the application as a user database.

## Database Checker

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



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

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



Also see the Database Manager User Guide.

---

## Changing Global Settings

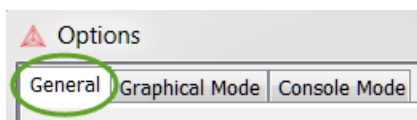
In the **Options** window (select **Tools** → **Options**) you can globally set general settings for Graphical Mode as well as default settings for any new activities for both Graphical Mode and Console Mode.

In this section:

---

<i>General</i> .....	<i>188</i>
<i>Graphical Mode - Default Units</i> .....	<i>189</i>
<i>Graphical Mode: Activities</i> .....	<i>190</i>
<i>Global Settings: Graphical and Console Mode-Plotting</i> .....	<i>200</i>
<i>Global Settings: Console Mode Default Appearance</i> .....	<i>203</i>

## General



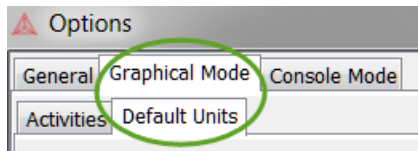
These settings are for both Graphical and Console modes. To open this window, from the main menu select **Tools → Options**.

### General Global Settings

Setting	Options
Tooltips enabled	Select whether to turn on tooltips information. By default the <b>Tooltips enabled</b> check box is selected. This displays a small text box when you hover the cursor above some buttons or other items.
Localization	To change the GUI language from the <b>Localization</b> list choose <b>English</b> (the default), <b>Swedish</b> , <b>Spanish</b> , <b>German</b> , <b>Russian</b> , <b>Chinese</b> , <b>Japanese</b> or <b>French</b> .
Look and feel	To change the <b>Look and feel</b> of the GUI layout, choose <b>Windows</b> (the default), <b>Metal</b> , <b>Nimbus</b> , <b>CDE/Motif</b> or <b>WindowsClassic</b> .
Database directory	<p>In the <b>Database directory</b> field, specify the path to the directory that contains the <b>data</b> directory. This is where the Thermo-Calc database directory called <b>data</b> is located. Do not specify the path to where the database files are found (that is, in the <b>data</b> directory).</p> <p><b>Modifying the Database Directory Path (Graphical Mode Only)</b></p> <p>Important Note: Database Directory Path (Graphical Mode only)</p> <p>When you open a database for the first time, it is stored in a cache (an intermediate storage area), that is maintained even if you close the program. This improves the speed of loading the next time you open that database. The cache is used for all databases that are listed in the database initialization file, typically all the standard databases that are included with Thermo-Calc.</p> <p>If you modify your own user-defined database, or if you choose to edit an unencrypted database, it is recommended that you create a separate directory to store these database files. This way the most recent version of the user-defined or edited databases are loaded into the program when the System Definer is performed.</p> <p>➤ Also see <a href="#">About the Database Files on page 184</a>.</p>

Setting	Options
Log level	Select the level and type of information to display in the <b>Event Log</b> window using the <b>Log level</b> slide bar. Choose from a <b>Debug</b> , <b>Info</b> , <b>Warning</b> or <b>Error</b> level of detail.
Check update interval	From the <b>Check update interval</b> list, choose not to check ( <b>Don't check</b> , the default) or <b>On startup</b> . You can also manually check for updates – choose <b>Help→Check for update</b> .
Reset to original settings	In the lower corner of the window, click the <b>Reset to original settings</b> button to restore the original settings. You may have to expand the window to view the button.

## Graphical Mode - Default Units

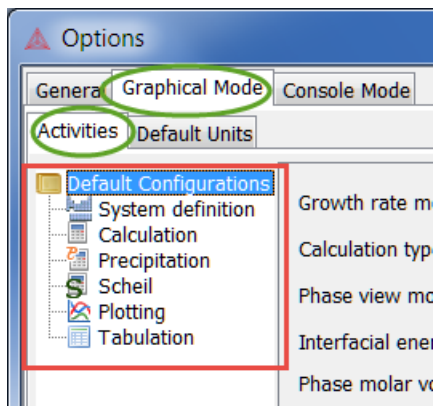


To open this window, from the main menu select **Tools → Options** and click the **Default Units** tab.

## Default Units - Settings in Graphical Mode

Setting	Options
Temperature	Kelvin (the default), Celsius or Fahrenheit
Pressure	Pascal (the default), Atmospheres or Bar
Amount	Mole (the default), Gram, Kilogram or Pound
Composition	Mass percent (the default), Mole percent, Mass fraction or Mole fraction
Energy	Joule (the default), Calorie or Electron volt
Volume	Cubic meter (the default), Cubic decimeter or Cubic centimeter
Density	Kilogram per cubic meter (the default) or Gram per cubic meter
Entropy	Joules per Kelvin (the default), Calorie per Kelvin or Electron volt per Kelvin
Length	Meter (the default), Micrometer or Nanometer
Time	Seconds (the default), Hours or Days
Reset to original settings	In the lower corner of the window, click the <b>Reset to original settings</b> button to restore the original settings. You may have to expand the window to view the button.

## Graphical Mode: Activities



To open this window, from the main menu select **Tools → Options** and click the **Activities** tab.

There are **System definition**, **Calculation**, **Precipitation**, **Scheil**, **Plotting** and **Tabulation** settings windows.

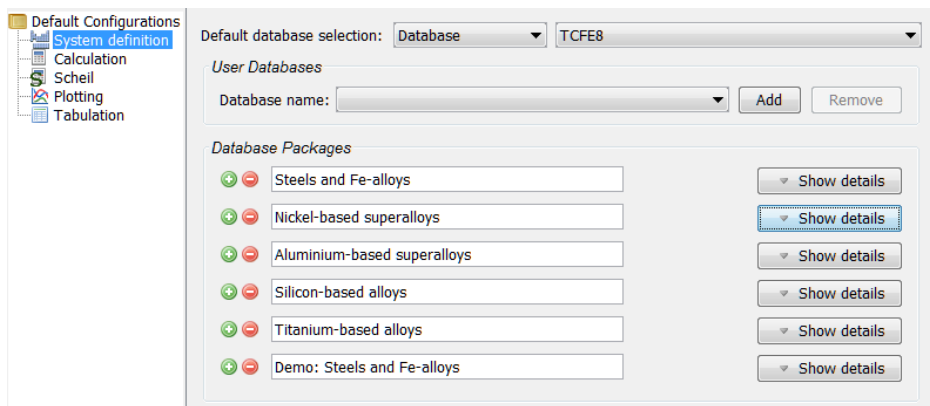


For Plotting, the default settings are shared with the Graphical and Console Modes. Any changes you make also apply to the default settings on the **Console Mode → Plotting** tab in the **Options** window (and vice versa). See [Global Settings: Graphical and Console Mode-Plotting](#) on page 200 for details.

## Global Settings: System Definition (System Definer)

When you create a new System Definer, the default databases are taken from these defaults. The database selections for each System Definer can then be configured individually. Once created, the specific (local) settings for a System Definer are not affected if you later make changes to the global defaults.




To open this window, from the main menu select **Tools → Options** and click the **Activities** tab. Then click **System definition**.





Also see [System Definer](#) on page 54, [Creating a Database Package](#) on the next page and [Clearing a Database Package Message](#) on page 193.

## System Definer Default Settings in Graphical Mode

Setting	Options
Default database selection	<p>Choose to define a <b>Database</b> or a <b>Database package</b>.</p> <p>If you choose <b>Database</b>, then select the default installed database to use globally for all System Definer nodes. For example, choose <b>TCFE8</b> or <b>TCNI8</b>.</p> <p>If you choose <b>Database Package</b>, select an option from the list. These Database Packages are defined in <i>Database Packages</i>.</p>
User Databases	

Setting	Options
Database name	<p>Click the <b>Add</b> button to add a custom database. After you have added the user database it is available from the list to choose as the default.</p> <p>Once a user database is added to the <b>Database name</b> list, you can also click the <b>Remove</b> button to delete it from your project.</p>
<b>Database Packages</b>	
Based on the installed databases, there are also default Database Packages available.	<p>Create and remove <b>Database Packages</b> by clicking the <b>Add a database package</b>  button or <b>Remove this database package</b>  button.</p> <div style="border: 1px solid black; padding: 10px; margin: 10px 0;">  The addition or removal of a database package does not take effect until a new System Definer node is defined. </div> <p>Click <b>Show details</b> to display the list of databases included with the package. Click <b>Hide details</b> to only display the name of the package. See <a href="#">Creating a Database Package</a> below.</p>
Reset to original settings	In the lower corner of the window, click the <b>Reset to original settings</b> button to restore the original settings. You may have to expand the window to view the button.

### Creating a Database Package

1. From the main menu select **Tools → Options**.
2. Click the **Activities** tab and click **System definition**.
3. Under **Database Packages**, click the **Add a database package**  button.
4. Replace the default text with a name for the package, for example **My database package**.
5. Select a database from the **Choose database** list, for example, **TCNI8**.
6. Click the **Add a database**  button and from the **Choose database** list, select another database, for example, **TCAL4**.
7. Click **OK**. The Database Package is now available to choose as the default for new System Definer activities.



The package is available for new System Definer nodes defined after adding the package.



*Clearing a Database Package Message below and [Global Settings: System Definition \(System Definer\)](#) on page 191.*

### *Clearing a Database Package Message*

Sometimes when working on the System Definer Configuration window, you may add or delete Databases. If you originally added a Database Package, the addition or removal of a database means that the original package you selected does not now match the databases you are using. To clear the message *Selected databases and selected package may differ* and reset the databases you need to either:

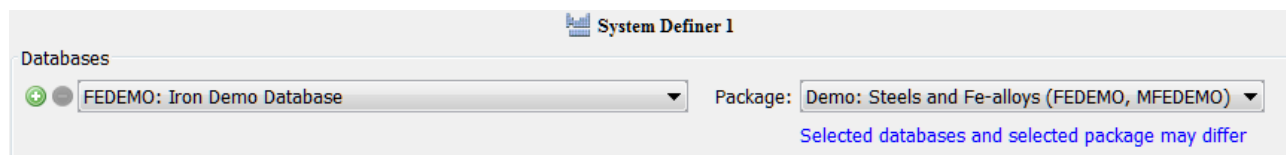
- Change the newly added database back to the one that matches the database package, or
- Choose another package from the **Package** list, then select the package you want.


For example, from the **Package** list you select **Demo: Steels and Fe-alloys**.

This adds the **FEDEMO** and **MFEDEMO** databases.



If you add or remove **Databases**, in this example **MFEDEMO** is removed, then this does not match the **Package** and the message displays:



To clear the message, click the **Add a database**  button and from the **Choose database** list, select the database that belongs with the package, in this example, **MFEDEMO**. The message is cleared.

You can also choose another package from the list, which changes the databases, and then re-select the original package to reset the message.



*Creating a Database Package on page 192 and Global Settings: System Definition (System Definer) on page 191.*

## Global Settings: Calculation (Equilibrium Calculator)

When you create a new Equilibrium Calculator, its initial settings are taken from these defaults. The settings of each Equilibrium Calculator can then be configured individually. Once created, the specific (local) settings for an Equilibrium Calculator are not affected if you later make changes to the global defaults.

To open this window, from the main menu select **Tools → Options** and click the **Activities** tab. Then click **Calculation**.



Also see *Equilibrium Calculator on page 72*.

These settings can also be changed locally for a certain Equilibrium Calculator.

Default calculation mode: **Simplified** Default calculation type: **Single equilibrium**

*Single Equilibrium and Property Grid*

☒ Global minimization

Max no of iterations: **500**

Max grid points  
**Coarse** **2,000**

Required accuracy: **1.0E-6**

Smallest fraction: **1.0E-12**

☒ Approximate driving force for metastable phases

☒ Force positive definite phase Hessian

☐ Control step size

*Property Diagram*

☒ Global minimization

Global test interval  
**Every 10th eq** **10**

*Phase Diagram*

☒ Global minimization

Global test interval  
**At node points** **0**

☒ Generate starting points automatically

☐ Use inside meshing points

No of meshes along an axis: **3**

### Equilibrium Calculator Default Settings in Graphical Mode

Setting	Options
Default calculation mode	Simplified (the default) or Advanced
Default calculation type	Single equilibrium (the default), Property diagram, Phase diagram or Property grid
<b>Single equilibrium and property grid</b>	
Global minimization	The check box is selected by default to ensure that the most stable minimum under the specified conditions is computed.
Max no of iterations	Default is 500
Max grid points	Coarse (2000 grid points, the default), Medium (20,000 grid points), Fine (200,000 grid points), or Custom (set your own number of grid points)
Required accuracy	The default is 1.0E-6
Smallest fraction	The default is 1.0E-12
Approximate driving force for metastable phases	The check box is selected by default

Setting	Options
Force positive definite phase Hessian	The check box is selected by default
Control stepsize	The check box is selected by default
<b>Property diagram</b>	
Global minimization	The check box is selected by default to ensure that the most stable minimum under the specified conditions is computed.
Global test interval	Every 10 <sup>th</sup> eq (the default), Always or Custom
<b>Phase diagram</b>	
Global minimization	The check box is selected by default to ensure that the most stable minimum under the specified conditions is computed.
Global test interval	At node points (the default), Every 10 <sup>th</sup> eq, Always or Custom
Generate starting points automatically	The check box is selected by default
Use inside meshing points	Click to select the check box as required
No of meshes along an axis	The default is 3
Reset to original settings	In the lower corner of the window, click the <b>Reset to original settings</b> button to restore the original settings. You may have to expand the window to view the button.

## Global Settings: Precipitation (Precipitation Calculator)

When you create a new Precipitation Calculator, its initial settings are taken from these defaults. The settings for each Precipitation Calculator can then be configured individually. Once created, the specific (local) settings for a Precipitation Calculator are not affected if you later make changes to the global defaults.

To open this window, from the main menu select **Tools → Options** and click the **Activities** tab. Then click **Precipitation**.



Also see [Precipitation Calculator](#) on page 78.

These settings can also be changed locally for a specific Precipitation Calculator.

## Precipitation Calculator Default Settings in Graphical Mode

Setting	Defaults/Options
Growth rate model	Simplified (default) or Advanced.
Calculation Type	Isothermal (default), Non-isothermal or TTT diagram.
Phase mode view	Hide details (default) or Show details
Interfacial energy	Calculated (default) or User-defined
Phase molar volume	Database (default) or User-defined.
Matrix grain size	1.0E-4 m (default)
Matrix grain aspect ratio	1.0 (default)
Dislocation density	5.0E12 m <sup>-3</sup> (default)
Nucleation sites	Bulk (default), Grain boundaries, Grain edges, Grain corners, or Dislocations.
Max time step fraction	0.1 (default)
No. of grid points over one order of magnitude in radius	150.0
Max no. of grid points over one order of magnitude in radius	200.0
Min no. of grid points over one order of magnitude in radius	100.0
Max relative volume fraction of subcritical particles allowed to dissolve in one time step	0.01
Max relative radius change	0.01
Relative radius change for avoiding class collision	0.5
Max overall volume change	0.001
Max relative change of nucleation rate in logarithmic scale	0.5
Max relative change of critical radius	0.1

Setting	Defaults/Options
Min radius for a nucleus to be considered as a particle	5.0E-10 m
Max time step during heating stages	1.0 s
Reset to original settings	In the lower corner of the window, click the <b>Reset to original settings</b> button to restore the original settings. You may have to expand the window to view the button.

### Global Settings: Scheil (Scheil Calculator)

When you create a new Scheil Calculator, its initial settings are taken from these defaults. The settings of each Scheil Calculator can then be configured individually. Once created, the specific (local) settings for a Scheil Calculator are not affected if you later make changes to the global defaults.

To open this window, from the main menu select **Tools → Options** and click the **Activities** tab. Then click **Scheil**.



Also see [Scheil Calculator](#) on page 108.

These settings can also be changed locally for a certain Scheil Calculator.

## Scheil Calculator Default Settings in Graphical Mode

Setting	Options
Start temperature	Enter a default <b>Start temperature</b> that is higher than the liquidus temperature of the alloy, in other words, the temperature at which the alloy is completely melted.
Temperature step	Enter a default <b>Temperature step</b> . Decreasing the temperature step increases the accuracy, but the default value is usually adequate.
Global minimization	By default the <b>Global minimization</b> check box is not selected. Click to select it to perform a global minimization test when an equilibrium is reached. This costs more computer time but the calculations are more robust.
Allow BCC → FCC	By default the <b>Allow BCC → FCC</b> check box is not selected. Select the check box to allow transformations in the solidified part of the alloy caused by each of the components specified to be a <i>fast diffuser</i> . It is recommended that you only select this for steels.
Reset to original settings	In the lower corner of the window, click the <b>Reset to original settings</b> button to restore the original settings. You may have to expand the window to view the button.

## Global Settings: Tabulation (Table Renderer)

When you create a new Table Renderer, its initial settings are taken from these default settings. The settings of each Table Renderer can then be configured individually. Once created, the settings of a Table Renderer are not affected by changes in the default settings. To open this window, from the main menu select **Tools → Options** and click the **Activities** tab. Then click **Tabulation**.



Also see [Table Renderer](#) on page 101.

## Table Renderer Default Settings in Graphical Mode

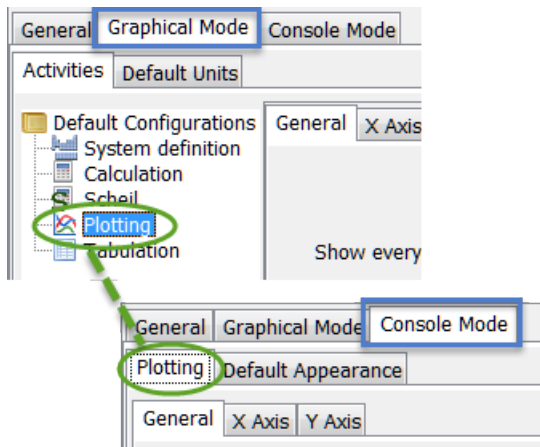
Setting	Options
Decimal digits	The default is 5
Number format	Auto (the default), Decimal or Scientific
Phase description detail	Composition (the default), Condensed, Constitution, or Composition and constitution

Setting	Options
Primary display color	Click <b>Modify</b> to change the default
Secondary display color	Click <b>Modify</b> to change the default
Reset to original settings	In the lower corner of the window, click the <b>Reset to original settings</b> button to restore the original settings. You may have to expand the window to view the button.

## Global Settings: Graphical and Console Mode-Plotting



The default settings are shared with both modes. Any changes you make also apply to the default settings on the **Console Mode → Plotting** tab in the **Options** window (and vice versa).



To make local changes to the appearance of a specific plot, in the **Results** window right-click a plot and select **Properties**. In the **Plot Properties** window a variety of settings can be made.

You can also edit some properties for individual plot lines (the color, the line width and type, and whether data points are included). In the **Results** window, hover the mouse over a plot line. The crosshair cursor turns into a cursor resembling a pointing hand when it is over a line that can be clicked. Alternatively, hold down Ctrl while you move the cursor around the plot to only display it as a crosshair and prevent unintended edits.

To globally configure the default settings for plotting, from the main menu select **Tools → Options**. Click the **Graphical Mode → Activities** tabs and then click the **Plotting** node.

When you create a new Plot Renderer, its initial settings are taken from these default settings. The settings can then be configured individually. Once created, the settings of a Plot Renderer are not affected by changes to the default global settings.

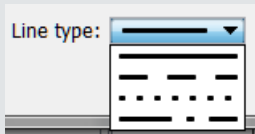
To configure the settings of an individual Plot Renderer rather than the default settings, right-click a plot in the **Results** window and select **Properties** from the menu.

### Plot Renderer Settings for Console and Graphical Modes

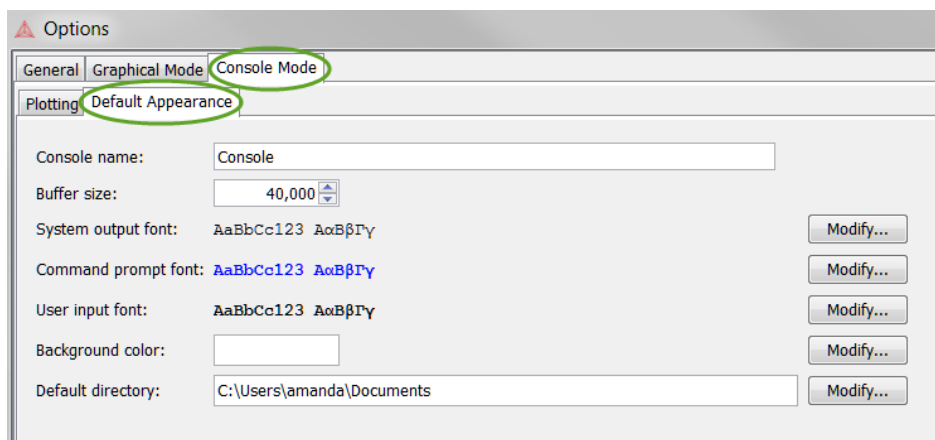
These global settings are available for both Console and Graphical Modes.

Setting	Options
<b>Title</b>	<p>Enter a title. Select <b>Plain text</b> (the default) or <b>LaTeX formatted text</b>.</p> <p>Click <math>\alpha</math> button to add symbols. Click a symbol category (for example, Latin characters or Greek and math symbols). Then click to choose the symbol located on the right-hand side.</p> <p>When you select <b>LaTeX formatted text</b> you can use the LaTeX math text to enter text. See <a href="#">ADD_LABEL_TEXT on page 190</a> and <a href="#">Adding and Editing Plot Labels on page 92</a> for more details.</p>
Title font, Legend font, Label font, Header font	Click <b>Modify</b> to edit the Font Name, Style, Size and Color.
Legend phase caption style	Choose <b>All</b> , <b>Constitution description</b> or <b>Ordering description</b> . See <a href="#">About Legend Styles on page 91</a> for details about these options.
Legend background color, Background color, Canvas color, Border color,	Click <b>Modify</b> to choose a color or enter a specific color.
Label format	Select Plain text (the default) or LaTeX formatted text.
Show anchor	By default, an anchor between the label and the plot point is displayed.
Retain labels (Graphical Mode only)	By default the check box is selected. Plot labels are kept (retained) when plots are updated. It can be applied globally or locally to individual plots.
Show header (Console Mode only)	Click to select the <b>Show header</b> check box to display the basic details about the plot along the top. This includes the date and time the plot is generated, the database used and the properties.
Border width	Choose a plot border width between <b>1</b> (thin, the default) and <b>10</b> (thick).
Color option	For the plot line colors, choose from the options in the list: <b>Legacy</b> , <b>Printer friendly</b> , <b>JFree chart</b> , <b>Pastel</b> , <b>Medium dark</b> , <b>Bright dark</b> , <b>Vivid</b> or <b>Earth</b> .



Setting	Options
	This option is also available for specific plot lines. To change the color of an individual plot line double-click it in the Results window and use the color palette to define it or enter a specific color.
Line width	For the plot line width, choose from the options in the list. These options are also available for specific plot lines. To change an individual plot line width double-click it in the Results window.
Line type	<p>This option is only available for individual plot lines. To change an individual plot line type double-click it in the Results window and choose an option from the list.</p> 
Show data points	Click to select the check box to display the data points on the plot lines. This option is also available for specific plot lines. To show data points on an individual plot line double-click it in the Results window and select the check box.
Data point marker size	Choose the data point marker size between <b>1</b> (small) and <b>10</b> (large). The default is 3.
Plot area size	The <b>Fit the plot area size to the enclosing window</b> option is selected by default. Excluding triangular plots, click Define the plot area size to enter a Plot area height and Plot area width.
Reset to original settings	In the lower corner of the window, click the <b>Reset to original settings</b> button to restore the original settings. You may have to expand the window to view the button.

## Global Settings: Console Mode Default Appearance



To open this window, from the main menu select **Tools → Options**. To change the name, buffer size, fonts and colours for a specific Console window, right-click the label for that particular Console and select **Properties**.

### Default Appearance Settings in Console Mode

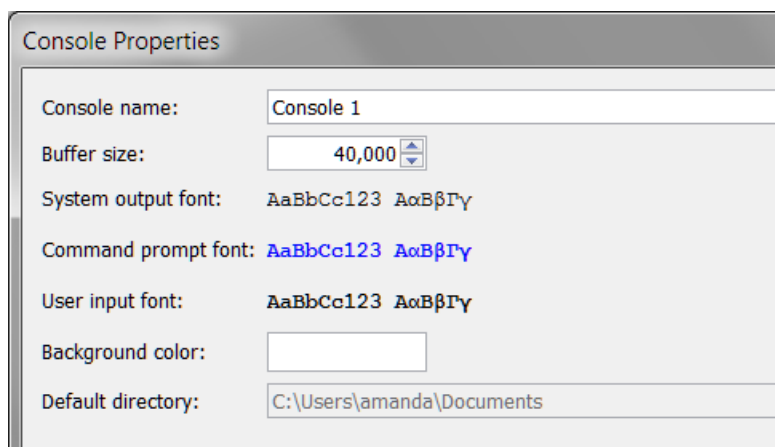
Setting	Options
Console name	The default is <code>Console</code> or enter another name to display
Buffer size	The default buffer size is 40,000.
System output font	Click <b>Modify</b> to open the <b>Select Font</b> window and makes changes to the font type, style, size or color as required.
Command prompt font	
User input font	
Background color	Click <b>Modify</b> to open the <b>Select Color</b> window to choose a background color for the Console Mode window where you enter commands.
Default directory	Set the default directory where log files and workspace files are saved.
Reset to original settings	In the lower corner of the window, click the <b>Reset to original settings</b> button to restore the original settings. You may have to expand the window to view the button.

### Increasing the Buffer Size

Sometimes the output overflows the window text buffer (see [Controlling Console Output on page 123](#)). To increase the buffer size in a specific Console tab:

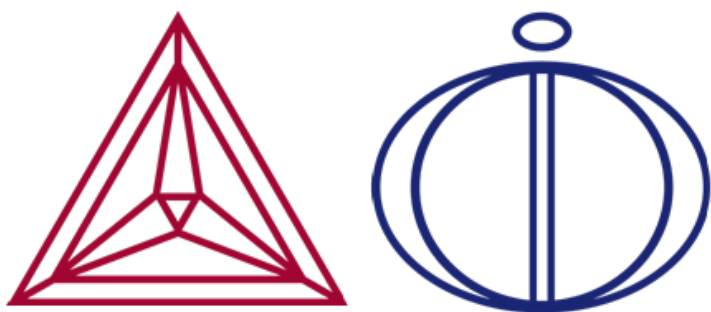
1. Right-click the Console tab header in the Console window (if this is the first Console tab, it is labelled **Console 1**).

2. Click **Properties**, and increase the **Buffer size** in the Console Properties window.



# **Console Mode Command Reference**

**Thermo-Calc Version 2016a**



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# Introduction to the Command Reference

In this section:

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<i>About the Console Command Reference .....</i>	<i>2</i>
<i>File Types .....</i>	<i>2</i>

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## About the Console Command Reference

This command reference is for Console Mode users of Thermo-Calc software. This guide describes the function and syntax of the commands available in the Thermo-Calc modules.



If you have the Diffusion Module (DICTRA) also see the *Diffusion Module (DICTRA) Command Reference* found in the Diffusion Module (DICTRA) Documentation Set PDF.

The commands available in all or most modules are described in the first topic ([General Commands on page 3](#)). The next topics are listed in alphabetical order based on the module names, then in each subtopic, the module commands.

### Abbreviations Used in this Guide

For the prompts, Y stands for Yes and N stands for No.

TC is for Thermo-Calc. For example, default file names often start with `tc.ini`.

## File Types



Also see the *Thermo-Calc Installation Guide* and the *Data Optimization User Guide* included with this documentation set for information about EXP files.

In Console Mode, Thermo-Calc uses different kinds of files, including:

- Log files (\*.LOG)
- Macro files (\*.TCM or \*.LOG)
- POLY workspace files (\*.POLY3)
- Experimental data files (\*.EXP)
- The GIBBS module uses a workspace file (\*.GES5)
- The PARROT module uses files with the suffixes \*.PAR and \*.POP.

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## General Commands

In this section:

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<i>BACK</i> .....	<i>4</i>
<i>EXIT</i> .....	<i>4</i>
<i>GOTO_MODULE</i> .....	<i>4</i>
<i>HELP (? and ??)</i> .....	<i>5</i>
<i>HELP</i> .....	<i>5</i>
<i>INFORMATION</i> .....	<i>5</i>
<i>MACRO_FILE_OPEN</i> .....	<i>5</i>
<i>SET_INTERACTIVE</i> .....	<i>8</i>

## BACK



Also see [GOTO\\_MODULE](#) below.

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

## EXIT

Syntax	EXIT
	Exit the program and return to the operating system. Use a save command before exiting otherwise all data and results are lost (in either the GIBBS, POLY, PARROT or REACTOR module).

## GOTO\_MODULE

Switch between modules. The name of the module must be typed. To get a list of available modules, press the <Enter> key.

Syntax	GOTO_MODULE
Prompt	MODULE NAME: <MODULE NAME>
	<p>If the &lt;Enter&gt; key is pressed without typing a unique module name (or typing a ? mark) it prompts for the MODULE NAME and lists the available modules</p> <pre> SYSTEM_UTILITIES GIBBS_ENERGY_SYSTEM TABULATION_REACTION POLY_3 DICTRA_MONITOR BINARY_DIAGRAM_EASY DATABASE_RETRIEVAL DIC_PARROT REACTOR_SIMULATOR_3 PARROT POTENTIAL_DIAGRAM SCHEIL_SIMULATION POURBAIX_DIAGRAM TERNARY_DIAGRAM MODULE NAME:            </pre>



## HELP (? and ??)

Gives text help about the current prompt (whether this is the prompt of a module, or a prompt that requests you to specify the value of some parameter).

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

## HELP

Lists the available commands or explains a specified command. Specifying a unique command displays an explanation on screen. Typing a command abbreviation that is not unique lists all matching commands. Get the command information by typing a unique abbreviation or the complete command name.

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

## INFORMATION

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

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

## MACRO\_FILE\_OPEN

The macro file functionality is a way to predefine sequences of Thermo-Calc commands stored in a macro file (a basic text file usually with the default extension TCM for the Thermo-Calc Console Mode or DCM for DICTRA module) and then executing all of the sequences using this command (preceded by the macro file name). This command can be used within various modules (i.e. the SYS, POLY, PARROT and TAB modules in the Thermo-Calc (Console Mode) software; SYS, POLY, PARROT and DICTRA\_Monitor).

Syntax	MACRO_FILE_OPEN
	<p>&lt;NAME OF A MACRO FILE *.TCM&gt;</p> <p>An <b>Open</b> window displays to specify the filename of the macro file (*.TCM) with the macro command, so that the path (in the <b>Look in</b> field) and <b>File name</b> can be specified.</p> <p>The <b>Files of type</b> *.TCM for Thermo-Calc (Console Mode) calculations and *.DCM for DICTRA simulations, cannot be changed. Click <b>Open</b> or <b>Cancel</b> to continue.</p> <p>If the macro file contains commands to set *.LOG files, to save or read GIBBS, POLY or PARROT workspaces, switch user databases, compile experiments (from existing *.POP files), create new *.PAR files, append *.EXP files, plot or dump diagrams, etc., a window (e.g. Save, Open, Print, etc.) displays on screen. If required, these windows can be avoided by issuing the file names (preferably with file-type extensions; if the files are not in the current working area where the macro is located, the appropriate and complete paths of the files should also be specified) and sometimes with the required options after the corresponding commands or parameters/options. For details, see the related commands and modules.</p> <p>When using a macro file that intended to plot graphs on screen, but the command <a href="#">SET_PLOT_FORMAT on page 210</a> is used to alter the plotting environment from the default value, it is important to first use the command SET_PLOT_FORMAT again to change back to the default value.</p>



See example 12 in the *Console Mode Examples Guide*.

This is useful when the same or similar calculations are made frequently with small changes [in terms of system definitions, data manipulations, conditions (for single points, stepping or mapping calculations), plotting settings, etc.]. For example, use this feature when calculating phase/property diagrams during an assessment of thermodynamic data.

A macro file can be automatically generated by the Thermo-Calc (Console Mode) software, if in the SYS module the [SET\\_LOG\\_FILE on page 242](#) command is used and a \*.LOG file name is given before any other SYS, DATA, TAB, GIBBS, POLY, POST, PARROT, or ED-EXP command or any special-module command (e.g. BIN, TERN, POTENTIAL, SCHEIL, POURBAIX, or REACTION). Such a \*.LOG file generated from the Thermo-Calc (Console Mode) software is a textual file, and using a textual editor (such as Notepad, WordPad, PFE, Emacs, vi, etc.) it can be edited, for example, by taking away unnecessary command lines, modifying some commands, settings and definitions, adding some pausing points, adding helpful commenting lines beginning with @@ signs, and so forth. Then save it as a macro file with the standard file extension TCM.

Experienced users can also write/edit an appropriate macro file for calculations/simulations, using any basic textual editor outside the Thermo-Calc program.

All commands can be used in a macro file. The file must be terminated with EXIT or be interrupted with SET\_INTERACTIVE.

Within a macro file you can use comment-lines (for describing the problems and for explaining commands and inputs/outputs), which should always start with the @@ signs in the beginning of each comment-line. Such comment-lines help to document the macro file, while these are not considered as command lines and thus do not affect the proceeding of all the normal commands in modules of the Console Mode when the file is called by the Thermo-Calc Console Mode software.

You can put multiple-line comment-blocks in a macro file between the @ (" and "@)" signs. The former sign indicates where the comment begins and the latter sign indicates where the comment ends. A comment-block begins from a line started with the *begin comment* sign @ (and ends with the *finish comment* sign @); all the lines written in between are ignored, and the line started with @) is also ignored.

Another use for a macro file is to allow you to interact at some specific points, using the "@?" sign starting a text line (note that the text describing the expected user-specification/input should be written as a continuous string without any empty space), for user's on-time specifications of arguments/parameters or inputs of parameter-values that are requested by a certain command. The macro temporally stops at the "@?" sign, prompt on screen the text given after "@?", and waits for the specified argument/parameter/value. The Thermo-Calc (Console Mode) software then uses specified argument/parameter/value as the input(s) for the associated command. For example, you can input the values of lower and higher temperature limits for the second axis-variable as follows:

```
GO POLY-3
SET-AXIS-VAR 2 T @?Low-temperature-limit:
@?High-temperature-limit:
```

You can have macro-variables denoted by the signs of @#n (for definition) and ##n (for usage); and up to nine variables inside a single macro file. Such a macro-variable can be assigned with its desired value, as for example:

```
@#3First-element?
```

This writes the text (note that the text describing the expected user specification/input is written as a continuous string without any empty spaces) after the "@#3" sign as prompted on screen and then wait for a specification. The input is assigned to the macro-variable ##3, which is directly called in different parts within the current macro file.

For example, the content of the macro-variable ##3 is inserted in the command:

```
DEFINE-SYSTEM ##3
```

It is also useful in more complicated commands, such as:

```
SET AXIS VAR 1 x(##3) 0 1,,,
```

This command sets the mole fraction of macro variable 3 as axis 1.

A macro file can have any number of pauses at the @& signs, for the purpose of checking the details/results of executing certain commands when running the macro file. However, you can also prevent the Thermo-Calc (Console Mode) software from temporarily stopping at any pause by typing any character (except for the Y character for confirming a Yes answer to a command prompt) after specifying the name of a macro file.

A macro file can have a maximum of five nested levels, i.e. a macro file can call another macro file, and if one sub-level macro is terminated by the command it resumes at the next command in the previous macro. If it is terminated by `end-of-file`, the Thermo-Calc (Console Mode) software stops.

This feature is especially useful for alloy design that requires many (hundreds) of calculations/simulations on similar material system/processes (specified in many different but appropriately-documented macro files that are organized in up to five levels) during a certain period of time (e.g. in an evening), you can run the main macro (on the top level) at a certain time (e.g. before leaving the office) and afterwards (e.g. next morning) you can systematically and efficiently check/compare/analyse the results (saved as graphical files, and/or EXP, TXT, XLS... files).

By adding the SYS command [SET\\_ECHO on page 242](#) at the beginning of a macro file (or in the primary macro file on the top level if any sub-level(s) of macro files are used), it is useful to automatically display the complete/detailed meaning of various commands in all the sequential operations in the software, all enforced according to the macro file(s).

## SET\_INTERACTIVE

Syntax	SET_INTERACTIVE
	Resets the input and output units to the initial values, i.e. keyboard and screen. Add this as the last command to the macro files.

---

## BINARY\_DIAGRAM Commands

In this section:

---

<i>BINARY_DIAGRAM Module</i> .....	<i>10</i>
------------------------------------	-----------

## BINARY\_DIAGRAM Module

The BINARY\_DIAGRAM module (short name, the BIN module) enables you to quickly calculate a simple binary phase diagram. Access to specific databases designed for BIN, such as TCBIN, is required.

To enter the module, at the SYS prompt type `GOTO_MODULE BINARY`. There are no other commands for this module. Follow the prompts to plot a diagram.



Also see the Graphical Mode equivalent to this command, [Binary Calculator](#) on page 104 in the *Thermo-Calc User Guide*.

Syntax	BINARY_DIAGRAM
Prompts	DATABASE: /TCBIN/
	FIRST ELEMENT SECOND ELEMENT
	PHASE DIAGRAM, PHASE FRACTION (F), G- OR A-CURVES (G/A): /PHASE_ DIAGRAM/

---

## DATABASE\_RETRIEVAL Commands

Search the online help or see in the *Thermo-Calc User Guide* for step-by-step instructions to define a system.

In this section:

---

<i>AMEND_SELECTION</i> .....	<i>12</i>
<i>APPEND_DATABASE</i> .....	<i>12</i>
<i>DATABASE_INFORMATION</i> .....	<i>13</i>
<i>DEFINE_ELEMENTS</i> .....	<i>14</i>
<i>DEFINE_SPECIES</i> .....	<i>14</i>
<i>DEFINE_SYSTEM</i> .....	<i>15</i>
<i>GET_DATA</i> .....	<i>15</i>
<i>LIST_DATABASE</i> .....	<i>16</i>
<i>LIST_SYSTEM</i> .....	<i>16</i>
<i>NEW_DIRECTORY_FILE</i> .....	<i>17</i>
<i>REJECT</i> .....	<i>17</i>
<i>RESTORE</i> .....	<i>18</i>
<i>SET_AUTO_APPEND_DATABASE</i> .....	<i>19</i>
<i>SWITCH_DATABASE</i> .....	<i>20</i>

---

## AMEND\_SELECTION

Use this command after defining the elements, species or the system (with the commands [DEFINE\\_ELEMENTS](#) on page 14, [DEFINE\\_SPECIES](#) on page 14, or [DEFINE\\_SYSTEM](#) on page 15). The prompts allow changes to the predefined system. By answering Y or N, each of the selected elements, species or phases can be accepted or rejected (although this is not the case for the constituents or the entire system).

Syntax	AMEND_SELECTION
Prompt	KEEP <NAME1> NO/QUIT /YES/ KEEP <NAME2> NO/QUIT /YES/
Options	KEYWORD-- ELEMENTS/SPECIES/PHASES NAME& Names of the pre-defined or pre-selected elements/species/phases

## APPEND\_DATABASE

Append data from a file or additional database to the current set of data already read from another database. Data already read from another database and stored in the Gibbs energy system is kept in the GES5 workspace.

This command also enters all additional parameters (phase constituents, G0 and interaction parameters, etc.) to already existing phases, and all existing parameters (phase constituents, excess model, G0 and interaction parameters, etc.) in the phase are replaced with the values retrieved from the appending database.

The command is equivalent to the SWITCH\_DATABASE USER command sequence. It is also similar to [SWITCH\\_DATABASE](#) on page 20, but does not reinitialize the DATA module and GIBBS workspace.

All the directly connected databases as predefined by the original database initiation file (TC\_INITD.TDB file in the /DATA/ area for Windows environments, or the `initd.tdb` file in the \data\ area for Linux), or by a user-specified database initiation file after using [NEW\\_DIRECTORY\\_FILE](#) on page 17, are listed after pressing <Enter> without giving any argument. You can supply your own database by giving the argument USER, the database name and the correct path if it is not located in the current working directory.

After the command is executed for the first time, the TDB\_XYZ: prompt (XYZ stands for the name of the primary switched database) is changed to the APP: prompt to go to more commands related to appending data.



Syntax	APPEND_DATABASE
Prompt	<p>Use one of these databases</p> <p>PURE    = SGTE PURE ELEMENT DATABASE</p> <p>SSUB    = SGTE SUBSTANCE DATABASE 1997</p> <p>USER     = USER DEFINED DATABASE</p> <p>DATABASE NAME /XYZ/: &lt;ADDITIONAL DATABASE NAME&gt;</p>
Options	<p>ADDITIONAL DATABASE NAME</p> <p>The name of an existing database or a USER database definition file (***)setup.TDB) that corresponds to the appending database.</p>
Notes	<p>If a USER database name or its path is not given on the same line of the APPEND_DATABASE command, or if the name or path is incomplete or incorrect, an Open window displays to open an appropriate database-setup. You can then open the USER database, or can cancel the open session; in the latter case, the program lists all predefined databases in the installation area, and you can select one of these or proceed with the USER option again for appending a desired database.</p> <p>When this command is used in a macro (*.TCM) file, if the USER option is selected, the database setup file name (*setup.TDB) containing the setup definitions of the USER database, and its correct path, are required.</p> <p>In Linux, the filename of a USER database, or one of the predefined names, can be used under the prompt <code>FILENAME:</code> This is a valid filename for the USER database definition file (***)setup.tdb) or a predefined database name, with the correct path. The default filename extension is <code>.tdb</code>.</p> <p>This command can be called more than once if appending two or more databases to the primary switched database.</p> <p>After this command, the commands to define a system (in terms of either elements or species), to reject/restore phases or species, and retrieve data must be repeated; however, the second keywords and parameter values might have to be different from the previous ones.</p>

## DATABASE\_INFORMATION


Syntax	DATABASE_INFORMATION
	<p>A short description of the current database is normally given by typing this command.</p> <p>This can include information on covered systems, used models, valid ranges for parameters in temperature and composition, major applications, and so on.</p>

## DEFINE\_ELEMENTS

Define the system in terms of elements. All possible species that can be formed by the given elements are retrieved from the database. The names of elements must be separated with a space or comma. It is possible to use a wildcard \* after a common part of element names so that all the elements, which start with that common part and are available in the currently switched or appending database, are defined in the system. Up to 40 elements can be defined into a single system.



Also see [Defining a System in Console Mode on page 127](#) in the *Thermo-Calc User Guide* for step-by-step instructions to define a system with this command.


Syntax	DEFINE_ELEMENTS
Prompt	<p>ELEMENT&amp; &lt;ELEMENT1, ELEMENT2, ...&gt;</p> <p>A list of elements to be defined into the system.</p>
	<p> When appending database(s), this command, or <a href="#">DEFINE_SPECIES</a> below or <a href="#">DEFINE_SYSTEM</a> on the next page must be repeated with the same or similar elements as defined in the first switched database.</p>

## DEFINE\_SPECIES

Define the system in terms of species. Only those species given are retrieved. The different names of species must be separated with a space or comma. It is possible to use a wildcard \* after a common part of species names so that all the species, which start with that common part and are available in the currently switched or appending database, are defined in the system. Up to 1000 species can be defined in a single system.



Also see [Defining a System in Console Mode on page 127](#) in the *Thermo-Calc User Guide*.

Syntax	DEFINE_SPECIES
Prompt	<p>SPECIES&amp; &lt;SPECIES1, SPECIES2, ...&gt;</p> <p>A list of species to be defined in the system.</p>
	<p> When appending database(s), this command, <a href="#">DEFINE_ELEMENTS</a> above or <a href="#">DEFINE_SYSTEM</a> on the next page must be repeated with the same or similar elements as defined in the first switched database.</p>

## DEFINE\_SYSTEM

Define the system in terms of either elements (equivalent to [DEFINE\\_ELEMENTS on the previous page](#)) or species (equivalent to [DEFINE\\_SPECIES on the previous page](#)). Certain databases have a default value of the keyword (as either ELEMENTS or SPECIES) reflecting what is most appropriate when defining a system.

The different names of elements or species must be separated with a space or comma. It is possible to use a wildcard \* after a common part of elements or species names so that all the elements or species, which start with that common part and are available in the currently switched or appending database, are defined in the system.

When appending database(s), this command (or DEFINE\_ELEMENTS or DEFINE\_SPECIES) must be repeated with the same or similar elements as defined in the first switched database. Different databases might contain different elements and have different species definitions: avoid defining elements/species that are missing in the appending database(s). Otherwise, the program indicates these missing elements/species, and ignores them in subsequent steps. But additional elements/species, and additional phases not available in the first switched database can be defined and retrieved from the appending database(s). Up to 40 elements and 1000 species can be defined in a single system.



Also see [Defining a System in Console Mode on page 127](#) in the *Thermo-Calc User Guide* for step-by-step instructions to define a system with this command.

Syntax	DEFINE_SYSTEM
Prompt	ELEMENTS: <ELEMENT1, ELEMENT2, ...>, OR SPECIES: <SPECIES1, SPECIES2, ...>
Options	Description
SPECIES OR ELEMENTS	Default keyword.
ELEMENT&	Specify a list of elements for the defining system.
SPECIES&	Specify a list of species for the defining system.

## GET\_DATA



Only after executing this command can you go to any of the application programs such as GES, POLY or DICTRA and use the retrieved data. When appending database(s), this command must be repeated in order to obtain the additional system definitions, parameters and functions.

Syntax	GET_DATA
	Enter the defined system's elements, species, phases, and the connected parameters obtained from either the primary switched or additionally appending database(s) to the GIBBS and/or DICTRA workspace. This command is necessary for retrieval of all information concerning a defined system from the databank.

## LIST\_DATABASE

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

Syntax	LIST_DATABASE
Options	Description
KEYWORD	One of the keywords Elements, Species, Phases or Constituent must be used to indicate what to list
ELEMENTS	All available elements, the reference state, atomic mass, H298-H0 and S298. Some elements have spaces in the column for the reference state. This implies that there are no parameters stored for this element.
SPECIES	All available species together with the stoichiometric factors.
PHASES	All available phases together with the number of sublattices and the number of sites in each sublattice.
CONSTITUENT	All available phases, the number of sublattices, the number of sites in each sublattice and the species dissolved in each phase. Species in different sublattices are separated with a colon (:). It is important to realize, for example, a phase can consist of Fe, Mo, V, and Cr, and its thermodynamic parameters can come from the binary systems Fe-Mo, Fe-V, Fe-Cr, and Mo-Cr. These data can give a relatively good description of the corners of the Fe-Cr-Mo system, but would most certainly give a bad one for the system Mo-Cr-V, due to the fact that the interaction parameters are, by default, set to zero, which originates from binary systems not included in the database.

## LIST\_SYSTEM

List all elements, species, phases or phase constituents in the defined system. It works only after a system is defined.

Syntax	LIST_SYSTEM
Keyword	One of the keywords Elements, Species, Phases or Constituent (as described in <a href="#">LIST_DATABASE</a> above) must be used to indicate what to list.

## NEW\_DIRECTORY\_FILE


Open a new database initiation file (or called database directory file) generated by a local database manager or user, for accessing additional databases not predefined in the original database initiation file.

The original database initiation file is automatically copied by the installation script to the main database area, on a local computer for an independent installation locates or a connected server for a server installation.

- For Windows this is the TC\_INITD (or TC\_INITD.TDB) file in the \DATA\ area under the directory defined by the TCPATH parameter.
- For Linux, it is the initd.tdb file in /data/ area that is under the directory defined by the TC\_DATA parameter. If the Thermo-Calc (Console Mode) is run on a Linux platform, the new database initiation file must be located in the current working directory.

If there are too many databases at one installation or if there are some user-specified databases for a particular purpose, a local database manager can generate additional database initiation files, or each user can have their own initiation file.

The command switches the working initialization of database groups in the DATA module among the original and additional database initiation files. The Thermo-Calc (Console Mode) can use additional database initiation files that define accessing paths to database groups (databases located in different subdirectories under the directory defined by the TCPATH or TC\_DATA parameter). All directly accessible databases remain as in the same group, until this command is called or recalled.

Syntax	NEW_DIRECTORY_FILE
Prompt	<p>FILE WITH DATABASE DIRECTORY /TC_INITD/: &lt;DATABASE-INITIATION-FILE NAME&gt;            ANOTHER DATABASE-INITIATION-FILE NAME</p> <p>The name of the next database initiation file (either additional or original) that is to be switched on as follows sessions.</p>
	<p> If the file name or its path is not given on the same line of the NEW_DIRECTORY_FILE command, or if it is incomplete or incorrect, an <b>Open</b> window displays to specify the new database initiation file.</p>

## REJECT

Reject elements, species, phases or phase constituents that can form from the defined elements and species. Phases/species/constituents that are possible to form in the defined system are removed from the list of system phases/species/constituents (shown by the command [LIST\\_SYSTEM](#) on the previous page). Phases/species/constituents that are not included in the list cannot be entered without first being restored. The different names must be separated with a space or comma. You can use a wildcard \* after a common part of names so that all the elements/species/phases/constituents that start with that

common part and are available in the currently switched or appending database, are rejected from the defined system.

This command can also reject a defined system, and thus reinitiate the entire DATA module memory and GES5 workspace.

Syntax	REJECT
Prompt 1	(keyword = ELEMENTS or SPECIES or PHASES) IF KEYWORD: <NAME1, NAME2, ...>
Prompt 2	(if keyword = CONSTITUENT) PHASE: <PHASE NAME> SUBLATTICE NUMBER: <SUBLATTICE NUMBER IN THE PHASE> CONSTITUENT: <CONSTITUENT(S) IN THE SUBLATTICE OF THE PHASE>
Prompt 3	If keyword = SYSTEM the DATA module is reset to its initial state; GIBBS is reinitiated and data already entered to GES5 is lost.
Options	Description and additional information
KEYWORD	One of the keywords <code>Elements</code> , <code>Species</code> , <code>Phases</code> , <code>Constituent</code> or <code>System</code> must be used to indicate what is rejected.
NAME&	Names of the pre-defined elements/species/phases/constituents/system
ELEMENTS	The given elements are rejected.
SPECIES	The given species are rejected, making it impossible to form them from the defined elements.
PHASES	The given phases are rejected, making it impossible to form them from the defined elements or species.
CONSTITUENT	The given constituent in one phase are rejected. Add the following when prompted: Phase: The name of the phase containing the constituent to be rejected. Sublattice number: The sublattice where the constituent enters (the first sublattice is 1). The question is omitted if there exists only one possible sublattice. Constituent: The name(s) of the constituent(s) to be rejected.

## RESTORE

Restore already explicitly rejected elements, species, phases or constituents; it is the opposite of the command *REJECT* on the [previous page](#) although it does not restore a completely rejected system.

Phases/species/constituents that are possible to form from the defined elements or species are entered to the list of system phases/species/constituents (shown by the command [LIST\\_SYSTEM](#) on page 16). Phases/species/constituents that are not included on the list can now be added to the list. The different names must be separated with a space or comma. It is possible to use a wildcard \* after a common part of names so that all the elements/species/phases/constituents, which start with that common part and are available in the currently switched or appending database, are restored in the defined system.

Syntax	RESTORE
Prompt1	(if keyword = ELEMENTS or SPECIES or PHASES) KEYWORD: <NAME1, NAME2, ...>
Prompt2	(if keyword = CONSTITUENT) PHASE: <PHASE NAME> SUBLATTICE NUMBER: <SUBLATTICE NUMBER IN THE PHASE> CONSTITUENT: <CONSTITUENT(S) IN THE SUBLATTICE OF THE PHASE>
Options	Description and Information
KEYWORD	One of the keywords <code>Elements</code> , <code>Species</code> , <code>Phases</code> or <code>Constituent</code> must be used to indicate what is rejected.
NAME&	Names of the pre-defined elements, species, phases, and constituents
ELEMENTS	The given elements are restored.
SPECIES	The given species are restored and thus possible to form from the defined elements.
PHASES	The given phases are restored and thus possible to form from the defined elements or species.
CONSTITUENT	The given constituent in one phase are restored. Add the following when prompted: Phase: The name of the phase containing the constituent to be restored. Sublattice number: The sublattice where the constituent enters (the first sublattice is 1). Constituent: The name(s) of the constituent(s) to be restored.

## SET\_AUTO\_APPEND\_DATABASE

Enforce an automatic action that appends thermodynamic data from a chosen database regarding the system to the data you already have about the system from the current database (that is, the default database or the database last chosen with [SWITCH\\_DATABASE](#) on the next page or [APPEND\\_DATABASE](#)

on page 12). This is useful to simultaneously retrieve both thermodynamic and mobility data for a defined system when performing a DICTRA module simulation.

This command should be used before defining a system (with the commands [DEFINE\\_ELEMENTS](#) on page 14, [DEFINE\\_SPECIES](#) on page 14, or [DEFINE\\_SYSTEM](#) on page 15) and retrieving the data with the [GET\\_DATA](#) on page 15 command from the primary switched database.

Syntax	SET_AUTO_APPEND_DATABASE
Prompt	DATABASE NAME /XYZ/: <ADDITIONAL DATABASE NAME>
Option	ADDITIONAL DATABASE NAME  The name of an existing database or a USER database that corresponds to the automatically-appending database.

It works in a way that is similar to the APPEND\_DATABASE<DATABASE-NAME> command sequence, but only the phases that are also available in the primary switched database are appended. There is no possibility to manually list, reject and/or restore any phase that is available in the appending database. When retrieving data with the GET\_DATA command afterwards, all the phases that exist in the appending database but not in the primary switched database are automatically rejected. The prompt is kept as for the primary switched database, TDB\_XYZ: (where XYZ stands for the name of the primary switched database) until the execution of the GET\_DATA command.

Therefore, to selectively append more phases from a secondary database to a system that is defined and retrieved from a primary switched database, then the APPEND\_DATABASE command and sequential commands (such as DATABASE\_INFORMATION, DEFINE\_SYSTEM, DEFINE\_ELEMENT, DEFINE\_SPECIES, LIST\_SYSTEM, REJECT, RESTORE and GET\_DATA) should be used instead, before this command.

Although it is impossible to manually list, reject and restore any phase from the appending database, the DATA module automatically ignores all the phases that do not exist in both the primary switched database and the appending database, and append the data for the phases (that are also available in the primary switched database) from the appending database, as informed on screen when executing [GET\\_DATA](#) on page 15 afterwards.

## SWITCH\_DATABASE

Switch (or change) from the current database to a new one, and reinitialize the entire DATA module for defining a system and the GES5 workspace for storing retrieved data. All the directly connected databases as predefined by the original database initiation file, or by a user-specified database initiation file after using [NEW\\_DIRECTORY\\_FILE](#) on page 17, are listed by pressing the <Enter> key without giving any argument. You can also supply your own database by giving the argument USER and then the database name and its correct path if it is not located in the current working directory. The second part of the prompt TDB\_XYZ indicates the present database XYZ.



<b>Syntax</b>	<b>SWITCH_DATABASE</b>
<b>Prompt</b>	<p>DATABASE NAME /XYZ/: &lt;NEW DATABASE NAME&gt;</p> <p>Use one of these databases:</p> <ul style="list-style-type: none"> <li>• PURE (SGTE pure element database)</li> <li>• SSUB (SGTE substance database 1997)</li> <li>• USER (user-defined database)</li> </ul>
<b>Options</b>	<b>Description and Information</b>
NEW DATABASE NAME	The name of an existing database or a USER database definition file (**setup.TDB).
DATABASE NAME	<p>The new database is specified by typing the abbreviation given in the front of one of the available predefined databases. When switching/appending databases or additionally purchased databases you can add these to the predefined database list in the database initiation file TC_INITD.TDB or initd.tdb of your installed software.</p> <p>When this command is used in a macro (*.TCM) file, if the USER option is selected, the database setup file name (*setup.TDB) that contains the setup definitions of the USER database, and its correct path, must be provided.</p>
FILENAME	In Linux, the filename of a USER database, or one of the predefined names, can be used under this prompt. A valid filename for the USER database definition file (**setup.tdb) or a predefined database name, with the correct path. The default filename extension is .tdb.
Notes	<p>If a USER database name or its path is not given on the same line of the SWITCH_DATABASE command, or if it is incomplete or incorrect, an Open window is displayed for the to-be-switched database.</p> <p>The USER database is used without reinitiating the Gibbs energy system, data from different databases can thus be combined. Therefore, the SWITCH_DATABASE USER command sequence is equivalent to the APPEND_DATABASE USER command sequence. The result of a combination must be examined carefully, because differences in standard states, phase models and names can be disastrous. If the same parameters occur in several such switched or appended databases, the last one retrieved is used in the calculations. It is not advisable to use this method for large databases since these load slowly.</p> <p>After this command, those commands for defining system (in terms of either elements or species), rejecting/restoring phases or species, retrieving data, as well as for appending data from additional database(s), can be proceeded.</p>

## EDIT\_EXPERIMENTS Commands



These commands are accessed through the PARROT module.

Some special commands are designed only for the ED\_EXP module and can also be used in \*.POP or \*.DOP files.

In this section:

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<i>Running the EDIT_EXPERIMENTS Command</i> .....	23
<i>COMPUTE_ALL_EQUILIBRIA</i> .....	23
<i>EXPERIMENT</i> .....	24
<i>EXPORT</i> .....	26
<i>IMPORT</i> .....	27
<i>LABEL_DATA</i> .....	28
<i>LIST_ALL_EQUILIBRIA</i> .....	28
<i>MAKE_POP_FILE</i> .....	28
<i>READ</i> .....	29
<i>RESTORE_ALL_WEIGHTS</i> .....	29
<i>SAVE_WORKSPACES</i> .....	30
<i>SET_ALTERNATE_CONDITION</i> .....	30
<i>SET_WEIGHT</i> .....	33
<i>STORE_ALL_WEIGHTS</i> .....	34
<i>TRANSFER_START_VALUE</i> .....	34

---

---

## Running the EDIT\_EXPERIMENTS Command

To run the EDIT\_EXPERIMENTS (ED\_EXP) module:

- The first necessary command after entering the ED\_EXP module for the first time (with [EDIT\\_EXPERIMENTS on page 95](#) in the PARROT module) should always be READ\_BLOCK in order to load the experimental data block from the current work \*.PAR-file for editing. Also, the read command must also be used prior to any other ED\_EXP command if the module is reinitiated, or if no experimental data block has not previously been read from a work file compiled with a proper experimental data .POP/.DOP file, or if you want to change to another data block for editing.
- If any change is made in the ED\_EXP module remember to use the command [SAVE\\_WORKSPACE on page 232](#) before going BACK to the PARROT module.



Although the TABLE\_HEAD, COMMENT and FLUSH\_BUFFER commands are visible in the ED\_EXP module, these cannot be used in the ED\_EXP module; these are only functional in an \*.POP or \*.DOP file.

## COMPUTE\_ALL\_EQUILIBRIA

In ED\_EXP and PARROT modules, each experiment is treated as an individual equilibrium with some measured values. These are created with [CREATE\\_NEW\\_EQUILIBRIUM on page 143](#), and stored in an experimental data \*.POP file and then compiled and saved in the POLY3 workspace of a PARROT work \*.PAR file.

With COMPUTE-ALL-EQUILIBRIA, all equilibria from the current to the last experimental points are calculated. If an equilibrium calculation fails, the calculation is stopped at that equilibrium. Equilibria with weight zero is skipped.



A current or present experimental point means the latest selected or calculated one. Once used the current point turns to the last point in the data block; in such a case you first use [SELECT\\_EQUILIBRIUM on page 162](#) so that the current point is switched to a desired one.

Syntax	COMPUTE_ALL_EQUILIBRIA
	<p>For this command there is always a list output on screen, which consists of six columns for all experimental points available in the current data block. The first column is the <i>equilibrium identifier</i> (a number) assigned by this command, the second the <i>data label</i> assigned with <a href="#">LABEL_DATA on page 28</a>, the third the <i>number of iterations</i>, the fourth the <i>current weight</i>, and the fifth the <i>current temperature</i>. In the sixth column the <i>fixed stable phases</i> are listed together with any <i>comment text</i> given after a <a href="#">COMMENT on page 40</a> in the *.POP or *.DOP file.</p> <p>If the weight is zero for an equilibrium columns 3-5 are replaced by the text <i>&lt;unused&gt;</i>. If the alternate mode is used for some experimental points, the listing is slightly different for such points. The 3-4 columns are displayed with <i>*alt*</i>, instead. If an alternate calculation is failed at one experimental point, the point is automatically assigned with a zero weight, and a warning message is shown above the data line (with all six columns).</p>

## EXPERIMENT

This command is used in original experimental data files (\*.POP or \*.DOP), but can also be given interactively inside the ED-EXP module, to change the value or uncertainty of an experiment or to add more experimental information.

An experiment usually consists of two parts with a colon (:) separating them:

- as a quantity relation, and
- as the uncertainty of the value for the quantity,

The quantity relation can be a normal POLY-module condition or an inequality (which is similar to condition but the relation between the quantity and given value is not in equality, i.e. < or >). The uncertainty can be expressed as an absolute value or relative to the value (x%).



An experiment that uses an inequality gives zero contribution to the sum of errors in the optimization procedure of PARROT if the value is on the right side. If the value is on the wrong side, the value after the colon determines how steeply the error increases with the value.

Syntax	EXPERIMENT
	<p>The experiment must be typed after the command. Several experiments can be given on the same line.</p> <p>The syntax of EXPERIMENT is similar to a CONDITION. Usually, a state variable set equal to a value with a given uncertainty is specified after the colon (:). For example, <math>T=1273.15:5</math>.</p> <p>An inequality, &lt; or &gt;, can also be used. For example: <math>ACR(C) &lt; -0.01:0.001</math>, <math>W(BCC, AG) &gt; 0.05:10\%</math></p>

## Additional Information About the EXPERIMENT Command

A typical experiment added interactively specifies that a phase should not be stable in a certain experiment, because a phase may appear in a range of composition or of temperature where it has never been observed during the optimization. A phase is unstable if its driving force is negative, and you can add experimental information to enforce that. For example, you can suppress the HCP phase in an existing experimental point:

```
CHANGE-STATUS HCP=DORMANT
EXPERIMENT DGM(HCP)<-.001:.0001
```



DGM is the POLY variable for the driving force that is already divided by  $RT$ , and it is dimensionless. Only dormant phases can have driving forces larger than zero, as this indicates that these would be stable if allowed to form. The experiment in the above case tries to modify the model parameters to make the HCP phase unstable.

More general examples of experiment definitions:

```
EXPERIMENT X(LIQ,PB)=.10:.01 X(FCC,PB)=0.02:.01
EXPERIMENT ACR(PB)=0.8:5%
EXPERIMENT T=700:5
```

The first experiment above describes a tie-line where the experimentally measured mole fraction of Pb is 0.1 in the liquid phase and 0.02 in the FCC phase, and its uncertainty is 0.01 for both measurements. The second experiment is that the activity of Pb should be 0.8 with an uncertainty of 5 percent.




The reference state of the component Pb must be set with the command [SET\\_REFERENCE\\_STATE](#) on page 169. The final one is that the temperature should be 700 K with an uncertainty of 5 degrees.

Experiments that are functions of states variable(s) must be described as the defined functions. For example:

```
ENTER_FUNCTION HTR=HM(LIQUID)-HM(FCC);
EXPERIMENT HTR=7000:1000
```

## EXPORT

Transfer/export a calculated value from an equilibrium to an optimizing variable in the PARROT workspace. Thus the value can be used, for example, in the Gibbs energy description of a phase. Of course, this variable should not be optimized (i.e. it should be set as a fixed variable in PARROT).

Syntax	EXPORT
Prompt	<p>FUNCTION NAME: &lt;FUNCTION NAME&gt;#&lt;N&gt;</p> <p>Specify the name of the function, the value of which should be transferred to a <math>\nabla</math> variable. The number (n) of the <math>\nabla</math> variable must be given after the function name, separated by hash character #.</p> <p> The function name is UPPER/lowercase sensitive, and it should normally be given in UPPER case.</p>
	<p><b>Example</b></p> <pre>ENTER_FUNCTION STRNGY=GM(FCC) .X(CU); EXPORT STRNGY#6</pre> <p>This transfers the value of the partial derivative of the Gibbs energy of the FCC phase with respect to the mole fraction of Cu to the optimizing variable 6 (i.e. <math>\nabla 6</math>).</p>

## IMPORT

Transfer/import the value of one of the optimizing variables to a constant. Normally, it is directly used inside an experimental data (\*.POP or \*.DOP) file. It is the inverse of [EXPORT on the previous page](#).


This is useful if several experiments are done at the same activity of a component, but this activity is not known. The activity should then be optimized and all equilibria with the same activity should use the same value. In this case the variable must be set as an optimizing variable, and an initial guess of the activity should be given. During the optimization, the PARROT program tries to find the activity that gives the best fit.



If an approximate value of the activity is known, it can be supplied as an experiment.



See example 36 in the *Console Mode Examples Guide*.

Syntax	IMPORT
Prompt	<p>CONSTANT NAME: &lt;CONSTANT NAME&gt;#&lt;N&gt;</p> <p>The value of the <math>v</math> variable must be assigned a symbolic constant. The number (<math>n</math>) of the <math>v</math> variable must be given after the constant name, separated by hash character #.</p> <p> The constant name is UPPER/lowercase sensitive, and it should normally be given in UPPER case.</p>
	<p><b>Example</b></p> <p>ENTER_CONSTANT ACU=0.1</p> <p>IMPORT ACU#2</p> <p>This transfers the value of the optimizing variable 2 (i.e. <math>v_2</math>) to the constant ACU.</p>

## LABEL\_DATA

Add a label to the experimental equilibrium point, either as a single point or several points given individually or in a table. The label is maximum four characters and must start with the letter A. Normally, it is directly used inside an experimental data (\*.POP or \*.DOP) file.

Several experimental equilibria can be given the same label, and the label can be used in the command [SET\\_WEIGHT](#) on page 33 to assign the same weight to all equilibria with the same label.

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

## LIST\_ALL\_EQUILIBRIA

Syntax	LIST_ALL_EQUILIBRIA
	<p>List all the details (including equilibrium indicators, labels, iteration numbers, weight, and fixed phases or comments) of all equilibrium points from the current one to the last one on screen. You can always use <a href="#">SELECT_EQUILIBRIUM</a> on page 162 to select a specific point as the current equilibrium point for such a list.</p>

## MAKE\_POP\_FILE

It is possible in the ED\_EXP module to make interactive changes and additions to the original experimental data file (the \*.POP or \*.DOP file).



To document or transfer the current or final experimental data to a \*.POP/\*.DOP file, you can use this command to write it to a new \*.POP/\*.DOP file or overwrite it on an old one.

Check this output carefully for errors. Tables in original \*.POP/\*.DOP files are written as individual experimental points. The output can be shown on screen or be saved as a new \*.POP file where to write or overwrite the edited experimental information in a simple text format.




If an existing \*.POP file name is specified, it is overwritten. In the DICTRA module, an \*.DOP file is written or overwritten.

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

## READ



This command must be given each time the ED\_EXP module is entered, unless it is already given once in ED\_EXP and does not use [LIST\\_RESULT](#) on page 104 or [OPTIMIZE\\_VARIABLES](#) on page 109 in PARROT in between.

Syntax	READ
Prompt	<p>BLOCK NUMBER /#/: &lt;N&gt;</p> <p>The number of data block that should be edited must be given. If there is no command <a href="#">FLUSH_BUFFER</a> on page 41 in the original POP or DOP file, then there is only one data block with the number 1.</p>
	<p> READ_WORKSPACE = READ</p> <p>This command (previously named READ_BLOCK) is equivalent to <a href="#">READ_WORKSPACE</a> on page 232 in the POLY module, but it only reads the POLY3 workspace from the work file set by <a href="#">SET_STORE_FILE</a> on page 116 in the PARROT module.</p>

## RESTORE\_ALL\_WEIGHTS

Restore a specific weight-set (previously saved by [STORE\\_ALL\\_WEIGHTS](#) on page 34) and assign all the different experimental points in the current data block with the previously-set weights in the sequential assessments.

Syntax	RESTORE_ALL_WEIGHTS
Prompt	SET NUMBER (0 FOR LIST) /0/: <WEIGHT-SET NUMBER> The default value 0 is for a list on screen.


## SAVE\_WORKSPACES

In the PARROT workspace this command saves the current status of the EDIT\_EXPERIMENT submodule before you switch back to the PARROT module. This is required when you want to save equilibria changes, including changes to conditions, experimental data, and/or computed equilibria results, as well as any newly added equilibria.

With this command all the changes made in the EDIT\_EXPERIMENT submodule are saved in the PARROT workspace. This means you do not need to execute [SAVE\\_PARROT\\_WORKSPACES on page 111](#) in the PARROT module.

However, when in the PARROT module, additional changes can only be saved with the SAVE\_PARROT\_WORKSPACES command even if they have been made prior to executing SAVE\_WORKSPACES in the EDIT\_EXPERIMENT module.

When you exit the EDIT\_EXPERIMENT module (or Thermo-Calc), the next time the file is opened it is in the same state as when you executed the SAVE\_WORKSPACES command. However, if you use [OPTIMIZE\\_VARIABLES on page 109](#) the computed results are automatically updated.

Syntax	SAVE_WORKSPACES
Prompt	<div> <div>&lt;FILE NAME&gt; &lt;Y OR N&gt;</div> <div>  Sometimes good starting values (<a href="#">SET_START_VALUE on page 171</a>) are required to successfully get or compute an equilibrium correctly. In this case, it is important to save the computed equilibrium in the PARROT workspace. It is important to remember that the computed results can be ruined by improper optimizations. For this reason, it is suggested you save the PAR file with a different name to back up the PARROT workspace. </div> </div>

## SET\_ALTERNATE\_CONDITION

A special command used in the experimental data \*.POP/\*.DOP file but also possible in the ED\_EXP module. It is used only when you have specified that the alternate mode is set in the PARROT module.


The command syntax is almost the same as for the POLY command [SET\\_CONDITION on page 165](#) while the uncertainty should also be specified.



The alternate condition (including the normally POLY-module condition plus uncertainty; see below) must be given explicitly, but can be given on the same line or on separate lines with each one started with the command.

Syntax	SET_ALTERNATE_CONDITION
Prompt	STATE VARIABLE EXPRESSION: <STATE VARIABLE NAME OR LINEAR EXPRESSION> Give either a state variable or a linear expression of state variables.
Options	<b>Description and Information</b>
State variables	<p>Some of the state variables that can be used in conditions are:</p> <ul style="list-style-type: none"> <li>• T (temperature in the system)</li> <li>• P (pressure in the system)</li> <li>• N (system size in moles)</li> <li>• B (system site in grams)</li> <li>• W(&lt;component&gt;) (mole fraction of a component in the system)</li> <li>• X(&lt;component&gt;) (fraction of a component in the system)</li> <li>• ACR(&lt;component&gt;) (activity of a component in the system)</li> <li>• MUR(&lt;component&gt;) (chemical potential of a component in the system)</li> <li>• W(&lt;phase&gt;,&lt;component&gt;) (mole fraction of a component in a phase)</li> <li>• X(&lt;phase&gt;,&lt;component&gt;) (mass fraction of a component in a phase)</li> <li>• ACR(&lt;phase&gt;,&lt;component&gt;) (activity of a component in a phase)</li> <li>• MUR(&lt;phase&gt;,&lt;component&gt;) (chemical potential of a component in a phase)</li> <li>• H (enthalpy in the system)</li> <li>• HM(&lt;phase&gt;) (enthalpy of a phase per mole)</li> </ul>
Additional prompts	<p>FACTOR: &lt;A FACTOR FOR THE STATE VARIABLE, OR A CONTINUATION&gt;</p> <p>This question means that the previous question was not answered. The program is then expecting a single state variable or a complete state variable expression, or the numeric factor in an expression with only one state variable. In a state variable expression a state variable may be preceded by a constant factor. An example of this is:</p> $2 * \text{MUR}(\text{FE}) + 3 * \text{MUR}(\text{O}) = -35000$ <p>This means that it should be a condition that two times the chemical potential of FE plus</p>


Syntax	SET_ALTERNATE_CONDITION
	three times the chemical potential of O should be -35000 J/mol.
	<p>STATE VARIABLE: &lt;A SPECIFIED STATE VARIABLE, OR A CONTINUATION&gt;</p> <p>This question is prompted if a single state variable name has not given in either the prompt <code>State variable expression</code> or <code>Factor</code>, or a state variable expression is given but the expression is incomplete, for example, <code>T-</code> or <code>2*MUR (FE) +</code>, for which the program is then expecting a continuation of the unfinished expression. You need to specify a state variable or a complete state variable expression, or complete the unfinished state variable expression. If a numeric factor is given before this prompt, only one state variable can be specified; otherwise, the program only takes the first state variable to complete the expression (i.e. the factor times the state variable).</p>
	<p>VALUE /X/: &lt;A NUMERIC VALUE, A CONSTANT OR A VARIABLE&gt;</p> <p>The value of the condition. This can be a numeric value, a constant or a variable. A suggestion is given as the default value. The special value <code>NONE</code> means that the condition is removed.</p>
	<p>UNCERTAINTY /NONE/: &lt;UNCERTAINTY OF THE CONDITION&gt;</p> <p>The uncertainty of the condition. This can be a numeric value, a constant or a variable. The default value <code>NONE</code> means that the uncertainty for the value specified above is zero. The uncertainty can either be expressed as an absolute value or relative to the value of the condition in percent (<code>x%</code>).</p>
Notes	<p>There are more state variables that can be used in conditions. For more information, type an <code>INFO STATE_VARIABLES</code> command in the POLY module. A condition is normally a value of a single state variable with its value.</p> <p><b>For example:</b></p> <pre>T=1273.15  P=1E5 X(C)=.002 W(CR)=1.5 ACR(CR)=0.85 X(FCC,C)=.001 H=-250000 HM(BCC)=-225000</pre> <p>A condition can also be a value of a linear expression involving more than one state variable.</p> <p><b>For example:</b></p> <pre>X(LIQ,S)-X(PYRR,S)=0</pre>


Syntax	SET_ALTERNATE_CONDITION
	<p>This means that it is a condition that the mole fraction of <i>S</i> should be the same in the LIQUID and PYRRHOTITE phases. In practice that should be the congruent melting point.</p> <p> After the equal sign only a numeric value is allowed.</p>



## SET\_WEIGHT

Each experimental value has an uncertainty associated with it, specified by the value after the colon (:) with the command [EXPERIMENT](#) on page 24. During an optimization the absolute difference between the experimental and calculated values gives a contribution to the sum of error.

With the SET\_WEIGHT command, you can change the scale of such a contribution (the uncertainty) for a single experimental point, or the contributions (all uncertainties) for a set of equilibria. The default weight is always unity. A value smaller than one means that the experiments should have less weight. A value larger than one that these should have higher weight. The special value zero means that the set of equilibria should be ignored in editing in ED\_EXP (as [COMPUTE\\_ALL\\_EQUILIBRIA](#) on page 23 is given) and in [OPTIMIZE\\_VARIABLES](#) on page 109 in PARROT.

-  The weight may be needed to obtain a balance between different kinds of experiments. For example, if there are only five experimental values of the composition of a phase diagram but 500 experimental values of activities or enthalpies, then the five composition points may have to be given higher weight than unity, otherwise these are not well described by the optimizing procedure.

Syntax	SET_WEIGHT
Prompts	<p>VALUE /1/: &lt;WEIGHT VALUE&gt;</p> <p>Specify a weight of the experiments in the specified equilibria (asked in the next prompt). The contribution to the sum of errors of these experiments are multiplied by this weight.</p> <p> The weight is squared, thus use 0.7 to make the error half (0.49) as big, and 1.4 to make it twice (1.96) as large.</p>
	<p>EQUILIBRIA (RANGE) OR LABEL(S) /PRESENT/:&lt;SELECTION&gt;</p> <p>Define the equilibria. These are available in the read data block from the current work file and are given the above-defined weight.</p> <p>The selection may be given as a range but the equilibrium numbers must then be separated only by a minus sign.</p>

Syntax	SET_WEIGHT
	<p> The start and end equilibrium numbers must be available in the read data block read from the current work file.</p> <p>For example, 5-101, means that all equilibria starting from the identifier 5 until the identifier 101. Some of numbers between these two identifiers may not exist in the data block.</p> <p>The selection may also be given as one or more labels (which should be separated only by a space). All equilibria with the specified label(s) in the read data block are given the above-defined weight.</p> <p>By pressing &lt;Enter&gt; to accept the default value <code>present</code>, the above defined weight is only assigned to the current or present experimental point (which is selected by the POLY command <a href="#">SELECT_EQUIBRIMUM</a> on page 162).</p> <p> If <a href="#">COMPUTE_ALL_EQUIBRIMA</a> on page 23 is used but no specific equilibrium point is selected afterwards, the last point in the read data block remains the <code>present</code> point.</p>

## STORE\_ALL\_WEIGHTS

Store a new weight-set that is the current situation of specified weights for all the different experimental points read from the currently-selected experimental data block in an assessment. This is useful when you want to try various weight-settings for some experimental points or for all the points, and then compare the assessment results from different weight-sets. Such a saved weight-set can be recalled and restored for all experimental data point with [RESTORE\\_ALL\\_WEIGHTS](#) on page 29 sequentially.

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

## TRANSFER\_START\_VALUE

In the ED\_EXP module it is time consuming to calculate all equilibria when the optimization is sensitive to start values of the composition of the phases. Usually in one data block there are several experimental points with the same kind of equilibrium and each must have its start value set. When you manage to calculate equilibriums of such experimental points, this command is useful to transfer the site fractions from a successfully-calculated equilibria to the present experimental point.

---

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

---

# Experimental Data Files

In this section:

---

<i>Commands in the Experimental Data Files (*.POP, *.DOP)</i> .....	37
<i>TABLE_HEAD, TABLE_VALUES and TABLE_END</i> .....	39
<i>COMMENT</i> .....	40
<i>FLUSH_BUFFER</i> .....	41



## Commands in the Experimental Data Files (\*.POP, \*.DOP)

In order to conduct an assessment for a system, the experimental data is described with a syntax, which is similar to the way that one calculates an equilibrium in the POLY module or you edit an experimental point in the ED\_EXP module. Similar to a Thermo-Calc (TCC) macro file (\*.TCM), an experimental data file (i.e. the \*.POP or \*.DOP file) is a basic text file and can be opened and edited by any text editor. For this reason, an \*.POP or \*.DOP file is not hardware dependent.

A POP or DOP file consists of various commands from the POLY and ED\_EXP modules, as well some special commands which can only be used in such experimental data files. Various experimental information can be inputted in an \*.POP or \*.DOP file as different tables; the same type of experimental data are usually documented in the same table (see below).

An \*.POP or \*.DOP file is used in the PARROT module to provide experimental information for the optimization process, and is checked by a *syntax checker* when the PARROT command [COMPILE\\_EXPERIMENTS](#) on page 92 is proceeded.

Many POLY and ED\_EXP commands can be directly used in a POP or DOP file. But there are some differences with the set of POLY or ED\_EXP commands, and some specially designed commands as described in this topic can only be used in the \*.POP or \*.DOP files.

### Frequently Used Commands

Most of the commands in the experimental data file are the same as in the POLY module. The most frequently used are listed below:

- [CREATE\\_NEW\\_EQUILIBRIUM](#) on page 143
- [CHANGE\\_STATUS](#) on page 135
- [SET\\_CONDITION](#) on page 165
- [SET\\_REFERENCE\\_STATE](#) on page 169
- [ENTER\\_SYMBOL](#) on page 195
- [SAVE\\_WORKSPACES](#) on page 30



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

### Other Commands

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

- [DEFINE\\_COMPONENTS](#) on page 143
- [EVALUATE\\_FUNCTIONS](#) on page 155

- [SET\\_ALL\\_START\\_VALUES](#) on page 162
- [SET\\_NUMERICAL\\_LIMITS](#) on page 168
- [SET\\_START\\_VALUE](#) on page 171
- [ADVANCED\\_OPTIONS](#) on page 125



The DEFINE-COMPONENTS command must be always used as the first command in an \*.POP or \*.DOP file, as it automatically reinitiates the whole workspace.

Most of the special commands for the ED\_EXP module are also often used in an \*.POP or \*.DOP file. For example:

- [EXPERIMENT](#) on page 24
- [EXPORT](#) on page 26
- [IMPORT](#) on page 27
- [LABEL\\_DATA](#) on page 28
- [SET\\_ALTERNATE\\_CONDITION](#) on page 30
- [SET\\_WEIGHT](#) on page 33



The following special ED\_EXP commands are illegal and should not be used in any \*.POP or \*.DOP file:

- COMPUTE-ALL-EQUILIBRIA
- MAKE-POP-FILE
- READ (READ-BLOCK OR READ-WORKSPACE)
- TRANSFER-START-VALUES

The special commenting identifier, i.e. a single dollar sign \$ which starts a line, is used to document comment lines at any position in an \*.POP or \*.DOP file. You may remember that this feature is universally the same as in almost all kinds of text files in Thermo-Calc software, e.g. in \*.TDB, \*.DAT, \*.TCM, \*.POP/\*.DOP and \*.EXP files. Such a sign and all information afterwards in the same comment line is skipped and ignored by the syntax checker. Therefore, you shall feel free to write such comment lines in any of these types of text files.

## TABLE\_HEAD, TABLE\_VALUES and TABLE\_END

These commands are used only in the \*.POP/\*.DOP files. It represents a convenient way to enter many experimental measurements of the same type in a table format.



These commands should always be used together and in a sequence, meaning that a table should always start with the TABLE-HEAD command, then follows the TABLE-VALUES command, and finish by the TABLE-END command. Between the two TABLE-HEAD and TABLE-VALUES commands, there should exist some definition lines (e.g. on phase status, reference states, conditions, experiments, labels, etc.) for the experimental measurements of the current information type.

Syntax	TABLE_HEAD TABLE_VALUES TABLE_END
Prompt	
	<p>After the TABLE-HEAD command, there must be an equilibrium description similar to a single experimental equilibrium but with some special notation. Then, there is always a TABLE-VALUES command, after which the actual data is given in columns. At the end of each table, there must be a TABLE-END command.</p> <p>The TABLE-HEAD command must be followed by a numeric value. This is used to generate unique numeric identifiers for all the equilibria in the table. The numeric identifier is incremented by one for each experimental (equilibrium) point in the table.</p>
	<p><b>Example</b></p> <p>An example of the use of a table for enthalpy measurements in the liquid is given here. Much more elaborate tables can be used</p> <pre>\$ Enthalpies of mixing, Topor and Kleppa, Met Trans 1984 TABLE-HEAD 1 CREATE-NEW @@ 1 CHANGE-STATUS PHASE LIQ=FIX 1 SET-REFERENCE-STATE AU LIQ * 1E5 SET-REFERENCE-STATE CU LIQ * 1E5 SET-CONDITION P=1E5 T=1379 X(LIQ,AU)=@1 LABEL ALH EXPER HMR=@2:5% TABLE-VALUES</pre>

Syntax	TABLE_HEAD TABLE_VALUES TABLE_END
	<pre> 0.0115 -322 0.0563 -1520 0.8499 -2976 0.9002 -2114 TABLE-END </pre>
	<p>The equilibrium description between TABLE-HEAD and TABLE-VALUES is similar as for a single experiment, except for these details:</p> <ul style="list-style-type: none"> <li>• @@ Used to automatically generate a series of identifying numbers instead of creating only one with the command <a href="#">CREATE_NEW_EQUILIBRIUM on page 143</a>. The program automatically generates the identifying numbers starting after the number given after the TABLE-HEAD command (in this case it is 1).</li> <li>• @1 values in the table are specified by an @ sign followed by a column number. In the above case, the mole fraction of Au in the liquid is in column 1 (see the line for SET-CONDITION). The columns may have other information than values, and you can use phase names or any text. If the text contains spaces or special characters, it must be surrounded by double quotes in the table, e.g. "ABC DEF&amp;ghi".</li> <li>• For the <i>syntax checker</i> all commands describing the equilibrium must be in UPPER case after the TABLE-HEAD command.</li> <li>• After the TABLE-VALUES command, there should be one line for each experimental measurement of the same type giving the values or texts that should be copied into the places of the condition or experiment defined by @1, t, etc. You can have columns that are not used but there must be exactly the same number of columns of each line, otherwise the syntax checker gives an error message in the PARROT module.</li> </ul>

## COMMENT

This command is only used in the \*.POP/\*.DOP files to write brief comments or descriptive information on a newly created equilibrium (experimental) data point or a set of points given in a table.

---

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

## FLUSH\_BUFFER

This command is only used in the \*.POP/\*.DOP files. It is needed if the number of experiments require more space than can be fitted into one buffer. When the PARROT program compiles experiments, it informs if any FLUSH commands are needed. The FLUSH\_BUFFER command terminates the current block, save it to the work file and starts a new block. With the READ command in the EDIT-EXP module, you can select the block to edit.

Syntax	FLUSH_BUFFER
	After a FLUSH_BUFFER command, the workspace is reinitiated and all functions or constants must be entered again in the *.POP file. You can take advantage of this; for example, you can use the FLUSH command to have blocks with different components in one *.POP file.

## GIBBS\_ENERGY\_SYSTEM Commands

In this section:

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<i>ADD_COMMENT</i> .....	43
<i>AMEND_ELEMENT_DATA</i> .....	43
<i>AMEND_PARAMETER</i> .....	44
<i>Solution Models in the GIBBS Module</i> .....	46
<i>AMEND_PHASE_DESCRIPTION</i> .....	52
<i>AMEND_SYMBOL</i> .....	57
<i>CHANGE_STATUS</i> .....	59
<i>ENTER_ELEMENT</i> .....	60
<i>About the ENTER_PARAMETER Command</i> .....	61
<i>ENTER_PARAMETER</i> .....	64
<i>About the ENTER_PHASE Command</i> .....	67
<i>ENTER_PHASE</i> .....	69
<i>ENTER_SPECIES</i> .....	71
<i>ENTER_SYMBOL</i> .....	72
<i>LIST_CONSTITUENT</i> .....	77
<i>LIST_DATA</i> .....	77
<i>LIST_PARAMETER</i> .....	78
<i>LIST_PHASE_DATA</i> .....	79
<i>LIST_STATUS</i> .....	80
<i>LIST_SYMBOL</i> .....	82
<i>READ_GES_WORKSPACE</i> .....	83
<i>REINITIATE</i> .....	83
<i>SAVE_GES_WORKSPACE</i> .....	84
<i>SET_R_AND_P_NORM</i> .....	85


---

## ADD\_COMMENT

Syntax	ADD_COMMENT
	Add a comment or make notes about parameters.

## AMEND\_ELEMENT\_DATA

The data for an element (in the SER, the Stable Element Reference, state) can be changed by this command. It should only be used for the elements that do not have any data in the database because the element data available in the database is set by the database-developer for the purpose of internal consistency. Except for the mass, the other values have no influence on the calculations.

Syntax	AMEND_ELEMENT_DATA
Prompts	<p>ELEMENT NAME: &lt;ELEMENT NAME&gt;</p> <p>Specify the name of the element for which you want to change the data.</p>
	<p>NEW STABLE ELEMENT REFERENCE /ABCD/: &lt;NAME OF SER&gt;</p> <p>Press &lt;Enter&gt; to accept the default SER or specify a new SER for the element. Important: The default name should not be changed if this data is retrieved from a database. This name is used when parameters for a phase are listed and the database assumes that the stable element reference is the same as in the database. Only if the element's data have not been fetched from a database, e.g. entered manually, can you enter a new SER.</p>
	<p>NEW ATOMIC MASS /XX.XXXX/: &lt;YYYYYY&gt;</p> <p>Press &lt;Enter&gt; to accept the default atomic mass or specify a new value for the element. The atomic mass of the element is given in g/mol.</p>
	<p>NEW H(298.15)-H(0) /XXX.XXX/: &lt;YYYYYY&gt;</p> <p>Press &lt;Enter&gt; to accept the default H(298.15)-H(0) or specify a new value for the element. H(298.15)-H(0) is the enthalpy difference between 298.15 K and 0 K for the element in its SER state.</p>
	<p>NEW S(298.15) /XX.XXXX/: &lt;YYYYYY&gt;</p> <p>Press &lt;Enter&gt; to accept the default S(298.15) or specify a new value for the element. S(298.15) is the absolute value of the entropy at 298.15 K for the element in its SER state.</p>
	<p>DEFAULT ELEMENT REFERENCE STATE SYMBOL INDEX /#/: &lt;INDEX&gt;</p> <div>  <p>The index only changes the symbol, not any value. Normally the index is set correctly by the database. Only when manually entering data, you must set the index to get the correct symbol.</p> </div>

Syntax	AMEND_ELEMENT_DATA
	<p>Specify an index for the default listing parameters (symbol), or press &lt;Enter&gt; to accept the pre-set index. 0 is for <math>G</math>, 1 is for <math>H_{298}</math> and 2 is for <math>H_0</math>.</p> <p>The index is to define the symbol printed in parameter listings. The symbol can be:</p> <ul style="list-style-type: none"> <li>• <math>G</math> the data are referred to Gibbs energy at a variable temperature (also called <i>lattice stability</i>).</li> <li>• <math>H_{298}</math> the data are referred to the enthalpy of the element at 298.15 K and 1 bar.</li> <li>• <math>H_0</math> is the same as <math>H_{298}</math> but at the temperature 0 K.</li> </ul>

## AMEND\_PARAMETER


Use this command to interactively change/amend the temperature-pressure function of a parameter. This is useful to correct typing errors because the old function is made available on the terminal for interactive editing. For most of these prompts, refer to [ENTER\\_PARAMETER on page 99](#) for details.

This AMEND\_PARAMETER command is for the GES module. There is also a PARROT module command with the same name ([AMEND\\_PARAMETER on page 88](#)).

Syntax	AMEND_PARAMETER
Prompts	<p>PARAMETER: &lt;PARAMETER NAME&gt;</p> <p>Specify a correct parameter name. If a parameter name is not acceptable or you only press &lt;Enter&gt;, the error message displays:</p> <p>ERROR, PLEASE RE-ENTER EACH PART SEPARATELY</p> <p>The program prompts for separate input for each part for a parameter name.</p>
	<p>IDENTIFIER (/X/): &lt;G OR L, OR TC, OR BM, OR V0 OR VA OR VB OR VC OR VK&gt;</p> <p>Specify one of these legal identifiers as described for ENTER_PARAMETER.</p>
	<p>PHASE NAME (/ABCD/): &lt;PHASE NAME&gt;</p> <p>Specify the phase name.</p>
	<p>CONSTITUENT (IN SUBLATTICE # /ABC/): &lt;SPECIES NAME&gt;</p> <p>Specify the constituent name.</p>
	<p>INTERACTING CONSTITUENT (IN SUBLATTICE # /XYZ/): &lt;SPECIES NAME&gt;</p> <p>Specify the interacting constituent name: If there is no interacting constituent, press &lt;Enter&gt;.</p>



Syntax	AMEND_PARAMETER
	<p>INTERACTING CONSTITUENT (IN SUBLATTICE # /XYZ/): &lt;SPECIES NAME&gt;</p> <p>If there are more than one interacting constituents, specify them; otherwise press &lt;Enter&gt;.</p>
	<p>DEGREE /#/: &lt;DEGREE&gt;</p> <p>Specify a numerical number as the degree of the phase parameter.</p>
	<p>After the parameter name is specified correctly, the program lists its current definition (either present in the database or defined by the ENTER_PARAMETER command), such as:</p> <pre>L (PHASE2,AL,MG;1)= 298.15&lt;T&lt;2000.00: +5000 2000.00&lt;T&lt;4500.00: +4500 4500.00&lt;T&lt;6000.00: +4000</pre> <p>Then you are prompted to change the parameter definition, as shown below:</p> <p>DO YOU WANT TO CHANGE THE NUMBER OF RANGES /NO/: &lt;Y OR N&gt;</p> <p>If you want to change the number of ranges for the chosen function, or change some of the temperature limits in the definition, for Y, retype both the low/high temperature limits and functions.</p> <p>If you do not want to change the number of ranges but want to change the function(s) in one or more ranges, press &lt;Enter&gt; to accept the default N, then the whole definition of the chosen parameter in all ranges (if any) is listed on screen, such as:</p> <pre>DIFFERENT FUNCTIONS IN THESE RANGES 298.15&lt;T&lt;2000.00 2000.00&lt;T&lt;4500.00 4500.00&lt;T&lt;6000.00</pre> <p>The prompt is given:</p> <p>DO YOU WANT TO CHANGE RANGE LIMITS /NO/: &lt;Y OR N&gt;</p> <p>If there is more than one range, this question is prompted press &lt;Enter&gt;.</p>
	<p>RANGE NUMBER (0 TO EXIT) /0/: &lt;RANGE NUMBER&gt;</p> <p>If the function of a parameter is different in two or more temperature ranges, you must specify the range of the function of which you want to amend. Or press &lt;Enter&gt; or type 0 to exit this command without making any changes.</p>
	<p>FUNCTION:</p>

Syntax	AMEND_PARAMETER
	<p>The previous function is available for editing. The editing is performed within the general subroutine FOOLED, as described in <a href="#">AMEND_SYMBOL on page 90</a>. This routine prompts as follows:</p> <pre>1:+:&gt;</pre> <p>The prompt consists of the current position in the string and the character at that position between colons, (::).</p> <p><b>Commands</b></p> <p>These commands can be given:</p> <ul style="list-style-type: none"> <li>• Help: ?</li> <li>• Move CP to last or first character: &lt;+/-&gt; A</li> <li>• Delete characters from CP: &lt;+-#characters&gt; D</li> <li>• Exit: E</li> <li>• Find: &lt;#occurrences&gt; F&lt;string&gt;@</li> <li>• Insert: I&lt;string&gt;@</li> <li>• Move: &lt;+-#positions&gt; M</li> <li>• Restore string: R</li> <li>• Substitute: S&lt;OLD&gt;@&lt;NEW&gt;@</li> <li>• Type string: T</li> </ul> <p>Where CP denotes the current position in string, # means number of, @ is a terminator of an input or search string.</p> <p> When the string is typed the character at the current position is replaced by an underscore _.</p> <p>To finish the editing of the current function, type E at the prompt.</p>

## Solution Models in the GIBBS Module

The command [AMEND\\_PHASE\\_DESCRIPTION on page 52](#) is used to specify/amend phase descriptions if a phase has a miscibility gap, uses a special excess energy model, or has a specific additional contribution to its Gibbs energy, for example.

This topic outlines the application of each option and includes important information about each command.

There are many solution models implemented in the GIBBS module (type `INFO MODELS` to see details about various thermodynamic models). However, these are switched on and handled differently via various GIBBS routines/commands:

- The first models the non-ideality as excess parts, i.e. by amending the phase's `EXCESS_MODEL` and/or `TERNARY_EXTRAPOLAT` models.
- The second models the non-ideality as `ADDITIONAL` parts, i.e. by amending the phase's other subjects in this command, e.g. `MAGNETIC_ORDERING` for the Magnetic Ordering Model, `DISORDERED_PART` for the CVM Approach in modelling chemical ordering/disordering phenomenon, `QUASICHEM_IONIC` for using a quasi-chemical entropy term for an ionic two-sublattice liquid solution phase, `QUASICHEM_FACT00` or `QUASICHEM_IRSID` for describing a substitutional liquid solution phase, `DEBYE_HUCKEL` for the DHLL/SIT Model in describing a dilute aqueous solution phase, etc.
- The third implements the model entirely or partially into the GIBBS module and related database(s), such as for the electrostatic contribution in an `AQUEOUS` solution phase by the Complete Revised\_HKF Model, the Murngham Model, Birch-Murngham Model or Generalized PVT Model for high-pressure/temperature volume contribution in a solid or liquid phase, the `SUPERFLUID` Model for the non-ideal EOS and non-ideal mixing in a gaseous mixture.

## NEW\_CONSTITUENT

Use this if you want to add a new constituent to a phase. It is illegal to add new constituents to an ionic two-sublattice liquid phase.

## RENAME\_PHASE

Use this to change the names of some specific phases. For example, a phase called `FE3O4_S` may be better named *Magnetite* to help identify it during the calculations and postprocessing. This is also a way to delete a phase by hiding it under a new name.

## SITE\_RATIOS

Use this to change the number of sites (i.e. the stoichiometric coefficients of various sublattices) in a sublattice phase.

## COMPOSITION\_SETS

Use this for solution phases that may have miscibility gap(s). However, this is less important today and often unnecessary to define additional composition set(s), since the implemented Global Minimization Technique can usually detect and add such composition set(s) in an automatic manner where it is really necessary during equilibrium calculations (of single-points, stepping or mapping).

## MAJOR\_CONSTITUENT

Use this to set major constituent(s) on each sublattice in each composition set for a solution phase. This

is useful to make calculations converge faster because it may simplify giving start values when calculating the equilibrium as those phases with miscibility gaps should have different major constituents for each composition set. The databases often set major constituents for several phases automatically when data are retrieved.

## FRACTION\_LIMITS

Use this to limit the application range (in terms of mole-fractions of all the involved elements) of a particular solution phase. This is useful to avoid automatic creations (enforced by the Global Minimization Technique) of additional composition sets for some solution phases (such as AQUEOUS solutions or dilute Fe-based liquid mixtures) of which the used models [e.g. the `SIT Model` or the `Complete Revised_HKF Model` for AQUEOUS solution, or the modified dilute solution parameters (plus a quadratic term, according to Hillert (1986) based on the SigworthElliot Model (Sigworth and Elliot, 1974) for Fe-rich liquid mixture] cannot be appropriately applied on a full scale.

Globally set the composition limits (in terms of mole fractions of various elements) in a specific solution phase, so that whenever the program finds a potential phase composition or a new composition set of possible miscibility gap(s) but that is out of this globally-set composition range, the program automatically ignores such a phase composition in an equilibrium calculation. This can be done either permanently inside a database (by enforcing this option for amending the phase-description of the solution phase) or temporarily within the GIBBS module (by using this phase-description amendment option).

This is important for solution phases for which the thermodynamic models and assessed data for the phases are for specific composition ranges, for example, the `FE_LIQUID` phase in the `SLAG` database is only applicable for Fe-rich liquid mixture, and the `AQUEOUS` phase in the `TCAQ/PAQ` and `AQS/PAQS` databases is only applicable for H<sub>2</sub>O-dominant aqueous solution phase.

Specify the low and high mole-fraction limits for each of the elements possibly available within the considered phase (in the currently defined system, or in a certain database). Do this for all the possible elements (defined in the phase) in a single `AMEND_PHASE_DESCRIPTION FRACTION_LIMITS` command-sequence, for example:

```
TYPE_DEFINITION R GES AM_PH_DES FE_LIQUID FRACTION_LIMITS Fe 0 0.6
    Ag 0 0.01  Al 0 0.05  Ca 0 0.05  Co 0 0.01  Cr 0 0.01
    Cu 0 0.02  Mg 0 0.05  Mn 0 0.05  Mo 0 0.05  Nb 0 0.05
    Ni 0 0.05  Pb 0 0.05  Si 0 0.10  Sn 0 0.02  Ti 0 0.05
U  0 0.01  V  0 0.02  W  0 0.02  Zr 0 0.03
    B  0 0.01  C  0 0.01  H  0 0.01  N  0 0.01  O  0 0.01
P  0 0.01  S  0 0.01  !
```

## DISORDERED\_PART

This command is needed for the special treatment of chemically-ordered phases where the contributions from the disordered state are described by a phase without ordering sublattices (the disordered phase name must be specified).

Several checks are made that the ordered and disordered phases are compatible (sublattices, sites and constituents). A link is then created between the phases, and the disordered phase is hidden from application programs. The Gibbs energy for the ordered phase also includes the Gibbs energy for the disordered phase.

Phases which can have an order/disorder transformation have parameters split on two phases and are referred to as the *two phase* description in the GIBBS module. One of them has sublattices for chemical ordering, the other one represents the disordered state. Normally, the ordered BCC and FCC or HCP phases may have either 2 or 4 substitutional sublattice (plus one additional interstitial site), that are handled by the Two Substitutional-Sublattice Ordering Model or Four Substitutional-Sublattice Ordering Model, respectively.

*Two phase* means that the *ordered* phase has parameters that describe the ordering. The *disordered* phase has all parameters for the reference state and those for describing the disordered phase. The ordered phase may occur only in some systems whereas the disordered phase may occur frequently, typical examples are the disordered FCC and BCC which may become ordered as L12 or B2 in certain systems. In order to treat multicomponent systems where some subsystems have ordering it would be necessary to transform all parameters of BCC into a B2 model.

The parameters describing the disordered phase are not changed but the Gibbs Energy system is informed that the Gibbs Energy for the two phases should be added.

The method used calculates the Gibbs Energy of a two phase model with two or four substitutional sublattices for ordering.

$$G_m = G_m^{ord}(y_i^I, y_i^II) + G_m^{dis}(x_i) - G_m^{ord}(y_i^I = x_i, y_i^II = x_i)$$



The mole fractions  $x_i$  are calculated from the site fractions  $y_i$ . The last term means that the contribution from  $G_m^{ord}$  in a disordered state (same site fraction, equal to the mole fraction, on both sublattices) is subtracted. The effect of this is that the parameters in the ordered phase have no contribution to the disordered state.

## MAGNETIC\_ORDERING

Change the magnetic ordering parameter for a certain phase with magnetic ordering contribution, in terms of its anti-ferromagnetic factor. By default this is -1 for BCC phase and -3 for all other phases (FCC, HCP, etc.). The fraction value of the total enthalpy (due to short-range ordering above the magnetic transition temperature) is by default 0.40 for BCC phase and 0.28 for all other phases (FCC, HCP, etc.).

## EXCESS\_MODEL

Use this to change the default Excess Model (for interaction energies) from the default (REDLICH-KISTER\_MUGGIANU). The model handles the excess interaction energies in a solution phase is chosen from:

- REDLICH-KISTER\_MUGGIANU: for binary (R-K) & ternary (R-K-M) interactions
- REDLICH-KISTER\_KOHLER: for binary (R-K) & ternary (R-K-K) interactions

- FLORY-HUGGINS POLYMER MODEL: for interactions in a polymer mixture phase (F-H)
- MIXED-EXCESS-MODELS: (R-K default) for mixed binary excess model (R-K, Legendre & Polynom) of a substitutional solution phase
- HKF: for interaction in an AQUEOUS solution phase (HKF)
- PITZER: for interaction in an AQUEOUS solution phase (PIT)
- CENTRAL\_ATOM\_MODEL: for interaction in a liquid slag solution phase (C-A-M)

For extrapolations of excess energies from related binary systems to ternary or higher-order systems, the Redlich-Kister binary excess interaction parameters may be extrapolated with either a Muggianu extension (i.e. the default REDLICH-KISTER\_MUGGIANU model) and a Kohler extension (i.e. the alternative REDLICH-KISTER\_KOHLER model), where there is no ternary, quaternary or higher-order interaction parameter.



The REDLICHKISTER\_KOHLER model is implemented only for ternary systems.

The MIXED-EXCESS-MODELS option works only for a substitutional phase with no sublattice (such as the metallic LIQUID phase) and it can be used to invoke asymmetrical simple or Legendre polynomial as binary excess energy models in addition to the default symmetrical Redlich-Kister model for the chosen pair of constituents in a substitutional phase with no sublattice. Asymmetrical here means that the power series depend only on one of the constituents, for example with expansions based on the  $[1-2 \cdot X(B)]$  term rather than  $[X(A)X(B)]$ .



Binary interaction parameters for such a pair of constituents must be entered prior to turning on the non-default Legendre or Polynom models.



See example 52 in the *Console Mode Examples Guide* for an example.

## TERNARY\_EXTRAPOLAT

Use this to change the extrapolation method from the default REDLICH-KISTER\_MUGGIANU to another extrapolation model. This method extrapolates from binary to ternary (and higher-order) excess interaction parameters in a solution phase and is chosen from:

- MUGGIANU for Muggianu Extrapolation from R-K parameters
- TOOP-KOHLER for Toop-Kohler Extrapolation Model
- KOHLER-ALL for Kohler Extrapolation Model
- MUGGIANU\_RESTOR for Muggianu-Restor Extrapolation Model



Only when all the relevant binary excess energies in the current solution phase are treated by the default Redlich-Kister Model (i.e. the Mixed-Excess-Model should have not been used), the MUGGIANU\_RESTOR method for ternary extrapolations is equivalent to the Redlich-Kister\_Muggianu Model, or the KOHLER-ALL method to the RedlichKister\_Kohler Model.

The default ternary extrapolation method MUGGIANU\_RESTOR applies to a solution phase as a whole, whatever the binary excess model(s) enforced to each of individual binary pairs in the phase. In case that all the binary pairs in the phase use the default binary excess model REDLICH-KISTER, then the ternary extrapolation method becomes the so-called Redlich-Kister\_Muggianu Model (in short as R-K-M), for extrapolations from binary parameters to ternary (and higher-order) excess energy terms; when no ternary L parameter is entered for that, such a default R-K-M Model is always used.

The KOHLER-ALL ternary extrapolation method can be turned on also for a solution phase as a whole, whatever the binary excess model(s) enforced to each of individual binary pairs in the phase. In case that all the binary pairs in the phase use the default binary excess model.

REDLICH-KISTER, then the ternary extrapolation method becomes the so-called Redlich-Kister\_Kohler Model (in short as R-K-K), for extrapolations from binary parameters to ternary (and higher-order) excess energy terms; when no ternary L parameter is entered for that, such an R-K-K Model is used.

The TOOP-KOHLER ternary extrapolation method is applied in a special way: for a specific ternary system (e.g. A-B-C) in a solution phase, specify which two constituents as the so-called Kohler constituents and the remaining constituent as the so-called Toop constituent on a given sublattice. If for the A-B-C ternary system you have specified A and B, or B and A, as the Kohler constituents (entered as the basis constituent and first interacting constituent) and C as the Toop constituent, only the A-B binary interaction parameters are used in accordance with the Kohler ternary extrapolation formula for A-B-C ternary interaction, while any other binary interaction parameters involving the Toop species C (i.e. of A-C and B-C binaries) are used in line with the Toop-Kohler ternary extrapolation formula (for the A-C-B and B-C-A ternary interactions).



This concept is shown in the *Console Mode Examples Guide*.

## DEBYE\_HUCKEL

To use the DHLL (Debye-Hückel Limiting Law) model and SIT (Specific Ionic Interaction Theory) model for a dilute AQUEOUS solution phase, switch the DEBYE\_HUCKEL part on, and it removes previously set (if any) ADDITIONAL part on the non-ideality for the chosen AQUEOUS phase.

## HKF\_ELECTROSTATIC

To use the hypothetical electrostatic contribution for the chosen phase (it must be an aqueous solution phase using the Complete Revised\_HKF Model). It removes previously set (if any) ADDITIONAL part on the non-ideality for the chosen AQUEOUS solution phase.

## QUASICHEM\_IONIC

To use the Quasichemical-Ionic model for the chosen liquid phase, you must have already entered/retrieved a liquid phase as an ionic two-sublattice liquid solution phase (normally, that is the IONIC\_LIQ phase), and then use this amending option to switch QUASICHEM\_IONIC on. It creates a completely new liquid solution phase [namely the QUAS\_IONIC phase which uses the Quasichemical Model for the entropy, according to Mats Hillert (2001: *J of Alloys and Compounds*, 320, 161-176)], while the original IONIC\_LIQ phase remains in the system and is not changed by this option.

### QUASICHEM\_FACT00

To use the Quasichemical Model developed by Kongoli et al. in the F\*A\*C\*T group in Montreal, you must have entered/retrieved a liquid phase using a normal substitutional liquid model with specified associates or species (on a single lattice site), and then turn on the option QUASICHEM\_FACT00. This removes the previously-set (if any) ADDITIONAL part on the non-ideality for the chosen liquid phase.



See examples 49 and 50 in the *Console Mode Examples Guide*.

### QUASICHEM\_IRSID

To use the Kapoor-Frohberg-Gaye Quasichemical Cell Model (i.e. the Quasichemical Model developed by IRSID, France) for a liquid SLAG solution phase, you can use a normal liquid model with specified associates or species.

### GLASS\_TRANSITION

To use the special model for glass transition of a liquid phase. It removes previously set (if any) ADDITIONAL part on the non-ideality for the chosen liquid phase.

### REMOVE\_ADDITION

To remove all the selected ADDITIONAL part from the Gibbs energy description for the chosen phase. If preferred, set a specific phase-status bit for a phase, use the PHASE\_BITS option as long you know the restrict meaning of each part of a phase- status bits.

### DEFAULT\_STABLE

Set phases as default-stable, which helps you to have a better guess of which phases that should be stable at the first calculation.



## AMEND\_PHASE\_DESCRIPTION

Specify/amend phase descriptions if a phase has a miscibility gap, uses a special excess energy model, or has a specific additional contribution to its Gibbs energy, for example.




Also see [Solution Models in the GIBBS Module on page 46](#) for detailed information about this command and its options.



Syntax	AMEND_PHASE_DESCRIPTION
Prompts	<p>PHASE NAME: &lt;PHASE NAME&gt;</p> <p>Specify the name of the phase.</p> <p>AMEND WHAT /COMPOSITION_SET/: &lt;SUBJECT&gt;</p> <p>Several subjects for the phase can be amended but most often this command is used to enter two or more composition sets for a phase. If a phase has a miscibility gap it is necessary to have two composition sets, one for each possible composition that can be stable simultaneously.</p> <p>Enter a question mark at the prompt to get a list of all possibly amended subjects for a phase.</p>
	<p>There are no additional prompts for DEBYE_HUCKEL, HKF_ELECTROSTATIC, GLASS_TRANSITION, QUASICHEM_FACT00, QUASICHEM_ISRID, REMOVE_ADDITION, and DEFAULT_STABLE.</p>
RENAME_PHASE	<p>NEW PHASE NAME /ABCD/: &lt;PHASE NAME&gt;</p> <p>Give a new phase name for the chosen phase, or press &lt;Enter&gt; to keep the default shown.</p>
SITE_RATIOS	<p>SITES IN FIRST SUBLATTICE /XX/ : &lt;YY&gt; SITES IN SECOND SUBLATTICE /XX/ : &lt;YY&gt;</p> <p>Specify the site numbers for each of the prompted sublattices for the current phase. Press &lt;Enter&gt; to accept the previous definitions.</p>
NEW_CONSTITUENT	<p>SUBLATTICE /#/: &lt;SUBLATTICE NUMBER&gt;</p> <p>Specify the sublattice where the new constituents are located.</p> <p>SPECIES: &lt;SPECIES NAME&gt;</p> <p>Give a valid species name.</p>
COMPOSITION_SETS	<p>NEW HIGHEST SET NUMBER /#/: &lt;SET NUMBER N&gt;</p> <p>The default value (#) is usually one higher than the current value. All phases have initially one composition set. If a lower value (i.e. lower than the default one) is given, that specific composition sets are deleted.</p> <p> You cannot take away the first composition set.</p> <p>MAJOR CONSTITUENT(S) FOR SUBLATTICE #: /AB/: &lt;MAJOR CONSTITUENT(S)&gt;</p> <p>Specify the new major constituent(s) for the sublattice #, or press &lt;Enter&gt; to accept</p>

Syntax	AMEND_PHASE_DESCRIPTION
	<p>the default which was automatically set according to the specified composition set of the phase.</p> <p>This prompt is repeated for all available sublattices in the chosen phase. The major constituents in each sublattice can be given. This may simplify giving start values when calculating the equilibrium as phases with miscibility gaps should have different major constituents for each composition set.</p>
MAJOR_ CONSTITUENT	<p>COMPOSITION SET /1/: &lt;COMPOSITION SET NUMBER&gt;</p> <p>Give the composition set (digit number) for the chosen phase, or press &lt;Enter&gt; if you want to set major constituents for the specified composition set.</p> <p>MAJOR CONSTITUENT(S) FOR SUBLATTICE #: /AB/: &lt;MAJOR CONSTITUENT(S)&gt;</p> <p>Specify the new major constituent(s) for the sublattice #, or press &lt;Enter&gt; to accept the default which is automatically set according to the specified composition set of the phase.</p> <p>This prompt is repeated for all available sublattices in the chosen phase for the specified composition set.</p> <p>The major constituents in each sublattice can be specified. This is useful in order to make calculations converge faster and more easily (because it may simplify giving start values when calculating the equilibrium as those phases with miscibility gaps should have different major constituents for each composition set). The databases often set major constituents for several phases automatically when data are retrieved.</p>
FRACTION_ LIMITS	<p>ELEMENT : &lt;EL1&gt;</p> <p>LOW FRACTION LIMIT /0/ : &lt;APPROPRIATE LOW LIMIT&gt;</p> <p>HIGH FRACTION LIMIT /1/ : &lt;APPROPRIATE HIGH LIMIT &gt;</p> <p>ELEMENT : &lt;EL2&gt;</p> <p>LOW FRACTION LIMIT /0/ : &lt;APPROPRIATE LOW LIMIT&gt;</p> <p>HIGH FRACTION LIMIT /1/ : &lt;APPROPRIATE HIGH LIMIT&gt;</p> <p>ELEMENT : &lt;ELN&gt;</p> <p>LOW FRACTION LIMIT /0/ : &lt;APPROPRIATE LOW LIMIT&gt;</p> <p>HIGH FRACTION LIMIT /1/ : &lt;APPROPRIATE HIGH LIMIT &gt;</p>
MAGNETIC_ ORDERING	<p>THE ANTIFERROMAGNETIC FACTOR /XX/: &lt;YY&gt;</p> <p>Specify the anti-ferromagnetic factor for the chosen phase. This should be –1 for BCC phase and –3 for all other phases (FCC, HCP, etc.).</p> <p>SHORT RANGE ORDER FRACTION OF THE ENTHALPY /XX/: &lt;YY&gt;</p>

Syntax	AMEND_PHASE_DESCRIPTION
	<p>The magnetic ordering is a second-order transformation and part of the enthalpy due to this transformation is due to short-range order. This value is the fraction of the total enthalpy that is due to short-range ordering above the magnetic transition temperature.</p> <p>The default value (xx) is 0.40 for BCC phase, and 0.28 for all other phases (FCC, HCP, etc.).</p>
DISORDERED_ PART	<p>DISORDERED PHASE NAME: &lt;PHASE NAME&gt;</p> <p>Give the disordered phase name for which there is no ordering sublattice.</p>
EXCESS_MODEL	<p>MODEL NAME /ABCDEFG/: &lt;MODEL NAME&gt;</p> <p>The default model is the pre-set model for the solution phase, normally the REDLICH-KISTER_MUGGIANU model, or choose another model for the phase to be amended:</p> <ul style="list-style-type: none"> <li>• REDLICH-KISTER_MUGGIANU</li> <li>• REDLICH-KISTER_KOHLER</li> <li>• FLORY-HUGGINS POLYMER MODEL</li> <li>• MIXED-EXCESS-MODELS (R-K default)</li> <li>• HKF</li> <li>• PITZER</li> <li>• CENTRAL_ATOM_MODEL</li> </ul> <p>The MIXED-EXCESS-MODELS option has sub-options:</p> <p>FIRST (THE INDEPENDENT) CONSTITUENT: &lt;CONSTITUENT NAME&gt;</p> <p>SECOND (THE DEPENDENT) CONSTITUENT: &lt;CONSTITUENT NAME&gt;</p> <p>Specify the binary pair of constituents in the current substitutional solution phase (the first one as the so-called independent constituent, and the second one as the dependent constituent), for which you wish to change the binary excess model from the default REDLICH-KISTER model to another model (LEGENDRE or POLYNOM).</p> <p>You are repeatedly prompted with the first sub-option (i.e. First (the independent) constituent after you have specified the desired binary Excess model type. To make further changes of binary excess model for other specific binary pairs in the current substitutional solution phase, press &lt;Enter&gt; (implying that there are no more changes of binary excess model for all other possibly-remaining binary pairs that shall still use the default REDLICH-KISTER model).</p> <p>EXCESS MODEL TYPE: /LEGENDRE/: &lt;DESIRED BINARY EXCESS MODEL TYPE&gt;</p>

Syntax	AMEND_PHASE_DESCRIPTION
	<p>For the currently-specified binary pair, choose one the legal binary excess models: LEGENDRE, POLYNOM or REDLICH-KISTER. If the default binary excess model REDLICH-KISTER is used for a certain binary pair, you can either specify the model name (or in short as R-K) or press &lt;Enter&gt;. After this sub-option, it returns to the first sub-option <i>First (the independent) constituent</i>: either for further change(s) of binary excess model of any other binary pair(s) or for termination (by pressing &lt;Enter&gt;) in the MIXED-EXCESS-MODELS option.</p>
TERNARY_EXTRAPOLAT	<p>EXTRAPOLATION METHOD: /TOOP-KOHLER/: &lt;TERNARY MODEL&gt;</p> <p>Choose a ternary extrapolation model for the current solution phase:</p> <ul style="list-style-type: none"> <li>• TOOP-KOHLER for Toop-Kohler Extrapolation Model</li> <li>• KOHLER-ALL for Kohler Extrapolation Model</li> <li>• MUGGIANU_RESTOR for Muggianu-Restor Extrapolation Model</li> </ul> <p>The TOOP-KOHLER option further prompts:</p> <p>CONSTITUENT IN SUBLATTICE #: &lt;BASIS CONSTITUENT NAME&gt;</p> <p>FIRST INTERACTION CONSTITUENT: &lt;INTERACTING CONSTITUENT NAME&gt;</p> <p>TOOP CONSTITUENT: &lt;TOOP CONSTITUENT NAME&gt;</p> <p>Specify the so-called Kohler constituents (entered as the basis constituent and first interacting constituent) and Toop constituent on a given sublattice in the current solution phase.</p>
QUASICHEM_IONIC	<p>To use the Quasichemical Model for the chosen liquid phase, you must first enter it as an ionic liquid phase, and then use this amending option. It creates a completely new phase, the original IONIC_LIQUID phase remains in the system and is not changed.</p> <p>NUMBER OF BONDS/ATOM /2/: &lt;NUMBER OF BONDS PER ATOM&gt;</p> <p>Specify the Z value (number of bonds per atom).</p>
STATUS_BITS	<p>Correct the phase status bits. It is important to fully understand this command before using it:</p> <p>NEW STATUS WORD (IN HEXADECIMAL) /04204000/: &lt;NEW STATUS BITS&gt;</p> <p> Also see <a href="#">LIST_STATUS</a> on page 80 for information on the status bits.</p> <p>Normally, these should never be changed in this way, because such phase status bits are automatically set on when all the phase descriptions (predefined in databases</p>

Syntax	AMEND_PHASE_DESCRIPTION
	and amended in the GIBBS module) are defined properly. The only exceptions are for the Kapoor-Frohberg-Gaye cell model for liquid SLAG solution phase, which can be set only as 04208000; and for the complete Revised HKF AQUEOUS solution model, which can be set as 02084000.

## AMEND\_SYMBOL

In the GIBBS and PARROT modules, interactively calculate the current values of a function or table (predefined by the switched database or previously entered with [ENTER\\_SYMBOL](#) on page 72) at the current temperature and pressure condition, and also possible to modify the definitions of variables or functions.




The current values of the temperature and pressure used to calculate the functions or tables are the ones listed with [LIST\\_STATUS](#) on page 80. There is no way to change the current temperature and pressure values interactively.

To modify the definitions of entered symbols (variable, functions or parameters), the performance of this command is slightly different one from another, as described below:

- For variables, the values can be changed.
- For functions the low and high temperature limits in various ranges (if any), as well the expressions, can be changed.
- For parameters the low and high temperature limits in various ranges (if any), as well the expressions, can be changed.

Syntax	AMEND_SYMBOL
Prompts	<p>NAME: &lt;SYMBOL NAME&gt;</p> <p>Specify the name of an entered symbol.</p> <p>For tables and functions (or parameters which are treated as functions after these are entered by the ENTER_SYMBOL command with the <code>Parameter</code> keyword, but not by the ENTER_PARAMETER command), after the symbol name is specified here, the program automatically calculates the values under the current temperature and pressure conditions, and lists the current values, such as:</p> <pre>FUNCTION VALUE  2.52500000E+01 TABLE VALUE    1.56000000E+02</pre> <p>For variables and functions (or parameters), there are additional prompts and depend on the symbol type.</p>
	<p>For a variable, its current value is displayed, and you can change it to a new value:</p> <p>VALUE /CURRENT VALUE/: &lt;NEW VALUE&gt;</p> <p>For a function (or a parameter entered as a symbol):</p> <p>DO YOU WANT TO CHANGE THE NUMBER OF RANGES /NO/: &lt;Y OR N&gt;</p> <p>To change the number of ranges for the function, or change some of the temperature limits in the definition, For <code>Y</code>, you must retype both the low/high temperature limits and functions (see all the remaining details in the ENTER_SYMBOL command.</p> <p>If you do not want to change it, press &lt;Enter&gt; to accept the default. The definition of the chosen function in all ranges (if any) is listed, for example:</p> <pre>DIFFERENT FUNCTIONS IN THESE RANGES 298.15&lt;T&lt;2000.00 2000.00&lt;T&lt;4500.00 4500.00&lt;T&lt;6000.00</pre> <p>and this message displays:</p> <pre>Do you want to change range limits /no/: &lt;y or n&gt;</pre> <p>If a function is different in two or more temperature ranges, you must specify the range of the function of which you want to amend. Or press &lt;Enter&gt; or type <code>0</code> to exit this command without making any change.</p>
	<p>RANGE NUMBER (0 TO EXIT) /0/: &lt;RANGE NUMBER&gt;</p> <p>FUNCTION:</p> <p>The previous function is available for editing. The editing is performed within the general</p>

Syntax	AMEND_SYMBOL
	<p>subroutine FOOLED. This routine prompts as follows:</p> <pre>1:+:&gt;</pre> <p>The prompt consists of the current position in the string and the character at that position between colons (::).</p> <p><b>Commands</b></p> <p>These commands can be given:</p> <ul style="list-style-type: none"> <li>• Help: ?</li> <li>• Move CP to last or first character: &lt;+/-&gt; A</li> <li>• Delete characters from CP: &lt;+-#characters&gt; D</li> <li>• Exit: E</li> <li>• Find: &lt;#occurrences&gt; F&lt;string&gt;@</li> <li>• Insert: I&lt;string&gt;@</li> <li>• Move: &lt;+-#positions&gt; M</li> <li>• Restore string: R</li> <li>• Substitute: S&lt;OLD&gt;@&lt;NEW&gt;@</li> <li>• Type string: T</li> </ul> <p>where CP denotes the current position in the string, # means number of, @ is a terminator of an input or search string.</p> <p> When the string is typed the character at the current position is replaced by an underscore _. To finish the editing of the current function, type E at the prompt.</p>

## CHANGE\_STATUS

For the GIBBS\_ENERGY\_SYSTEM Module, the status of an element or species or phase can be either ENTERED or SUSPENDED. The suspended status can be either implicit or explicit. The implicitly suspended status can be set e.g. for a species if any of the elements in its chemical formula is explicitly suspended. A species that is implicitly suspended becomes entered automatically if all its elements are set entered. After this command, a message shows which elements/species/phases are suspended or restored (entered). Consequently, the status bits for the specified elements or species or phases are changed, as listed with [LIST\\_STATUS](#) on page 80.

Syntax	CHANGE_STATUS
Prompts	<p>FOR ELEMENT, SPECIES OR PHASE /SPECIES/: &lt;KEYWORD&gt;</p> <p>Specify the keyword (element, species or phase).</p>
	<p>SUSPEND /Y/: &lt;Y OR N&gt;</p> <p>The status is changed from ENTERED to SUSPENDED (Y), or vice versa (N).</p> <p>If an element is suspended all species with this element become implicitly SUSPENDED too. A phase may become implicitly suspended if all its constituents or all constituents in a sublattice are suspended.</p>
	<p>LIST OF ELEMENTS/SPECIES/PHASES: &lt;NAME OF ELEMENTS OR SPECIES OR PHASES&gt;</p> <p>Specify the names or indices of those elements or species or phases that shall become suspended or active. For names, these should be separated by a space and terminated with a semicolon (;) or an empty line. For indices it is possible to give a range by separating two numbers by a hyphen (-). The list should be terminated by a semicolon (;). Example: 5 1 7-12 FE;</p>

## ENTER\_ELEMENT


Specify a system interactively. The program searches the currently switched or preset database for data for the given elements. The data for the elements in the database are the:

- mass in g/mol
- name of the Selected Element Reference State (SER) which normally is the stable phase for the element at 298.15 K
- enthalpy difference for the element in the SER state at 298.15 K and zero K
- absolute entropy for the element in the SER state at 298.15 K.

The two predefined elements, i.e. electrons and vacancies, have the chemical symbols /- and  $\text{v}_\text{A}$ , respectively. Initially, these are suspended but can be entered either by this command or [CHANGE\\_STATUS](#) on the previous page.

If an aqueous solution phase is involved, in the GIBBS module you enter a special aqueous electron called, ZE. This is specially designed for appropriately calculating the standard electric potential in the aqueous solution system.



Syntax	ENTER_ELEMENT
Prompt	<p>ELEMENT NAME: &lt;ELEMENT NAME&gt;</p> <p>Specify several elements on one line. The name of an element is its chemical symbol. The chemical symbols must be separated by spaces. Fictitious element names are legal but naturally no data are found in the database for them.</p>
	<p> An element name (maximum 2 characters) can either have its first letter in upper and the second (if any) in lower case (i.e. Lower Case Mode) or both letters can be in upper or lower case (i.e. Upper Case Mode). The Upper or Lower Case Mode is selected by the command <a href="#">REINITIATE</a> on page 83, which removes all data, and should be executed before any other command.</p>

## About the ENTER\_PARAMETER Command



For the PARROT Module, this command is the same and is described here. Also see [ENTER\\_PARAMETER](#) on page 99 for the command details.

In the descriptions of the standard thermochemical properties and special physical properties for a phase, there are a number of parameters which may depend on the temperature and pressure. The expressions for these parameters can be given in a free form as a sum of terms with powers of T and P and may also include the natural logarithm and exponential function. This type of expression is called *TP-functions*. Identical parameters (in terms of parameter-names) are stored only once in the GIBBS workspaces.

The composition-dependence of the Gibbs energy is described in the GIBBS module by the internal data structure, which is created when the phase is entered (see [GIBBS\\_ENERGY\\_SYSTEM Commands](#) on page 42). The Gibbs energy of a phase is always referred to one formula unit of the phase, i.e. the amount derived from the number of sites (i.e. the stoichiometric coefficient) for each sublattice. If vacancy is a constituent of a sublattice, the amount of matter per formula unit of the phase may vary with composition.

### Defining the Parameter

A valid parameter should have the general form of:

```
<identifier>(<phase>, <constituent array>; <digit>) <xxx> <expression> <yyy> <keyword  
Y or N> <zzz> !
```

The identifier must be followed by an opening parenthesis, a phase name, a comma and a constituent array. Optionally, the constituent array can be followed by a semicolon and a digit. The parameter name is terminated by a closing parenthesis. The parameter form is defined as:

- `<identifier>` is the parameter type;
- `<phase>` is the phase name (maximum 24 characters);
- `<constituent array>` is the specific constituent array in the phase;
- `<digit>` is the degree of composition-dependent interaction contribution (an integer number from 0 through 9), that is only for excess energy (L), Curie temperature (TC) and Bohr magneton number (BMAGN), as well as for volume-related parameters (V0 or VA or VB or VC or VK); if it is valued as zero, or if it is for the standard Gibbs energy (G) for which the degree is always zero, it can be omitted;
- `<expression>` is the mathematical relation to describe the parameter;
- `<xxx>` and `<yyy>` are the low and high temperature limits respectively for the applicable temperature range of the parameter expression;
- `<keyword Y or N>` is the indicator on if there is continuation for the parameter expression or not;
- `<zzz>` is the reference index/number for the assessment of this parameter;
- The exclamation point ! is used to indicate that the current parameter definition is ended.

## PARAMETER NAME

The GES parameter name has a general form of:

```
<identifier>(<phase>,<constituent array>;<digit>)
```

Examples of parameter names:

- `G (GAS, C1O2)` : The Gibbs energy of formation of a CO<sub>2</sub> molecule in gas.
- `G (FCC, Fe:VA)` : The Gibbs energy of formation of fcc Fe with interstitials.
- `L (LIQ, Fe, Cr; 0)` : The regular solution parameter for Fe and Cr in liquid.
- `L (LIQ, Fe, Cr; 1)` : The sub-regular solution parameter.
- `TC (BCC, Fe:Va)` : The Curie temperature of bcc Fe.
- `BMAGN (BCC, Fe:Va)` : The Bohr magneton number parameter of bcc Fe.

The parameter name consists of several parts. The first is a type-identifier and these can be used:

- **G**: Standard energy parameter (Gibbs energy of formation) or for interaction parameters;
- **L**: Excess energy parameter (Gibbs energy of interaction) always used for interaction parameters;

- TC: Curie temperature for magnetic ordering;
- BMAGN or BM: Bohr magneton number for magnetic ordering (or Born function  $\omega_{Pr,Tr}$  for aqueous solute species).
- VO: Molar volume at 298.15 K and 1 bar (a numeric value only);
- VA: Integrated thermal expansivity;  $\int_{298.15}^T \alpha(T) dT$
- VB: Bulk modulus at 1 bar;
- VC: Isothermal compressibility;
- VK: High-pressure fitting parameter.



When necessary quantities as  $H$  (enthalpy),  $S$  (entropy),  $V$  (Volume),  $F$  (Helmholtz energy), etc., can be calculated from the Gibbs energy.

## PHASE NAME

Specifying the PHASE NAME in uppercase is recommended; however, if you prefer to write it as a mixture of uppercase and lowercase, it automatically converts all lowercase to uppercase, as the GIBBS module only recognises uppercase phase names. It is important that if a phase bears a legal phase-type (among G, A, Y, L, I, F and B) in its phase definition (already by the PHASE keyword; such as GAS:G, LIQUID:L, SLAG:L, IONIC-LIQ:Y, SPINEL:I, FCC\_L12:F, HCP\_D021:F, BCC\_B2:B, AQUEOUS:A), such a valid phase-type code should not be attached to the phase name when ENTER\_PARAMETER is executed.

## CONSTITUENT ARRAY

The constituent array consists of a list of constituent names. Interaction parameters have two or more constituents from the same sublattice separated by a comma. If the phase has sublattices, at least one constituent in each sublattice must be specified. The constituents in different sublattices must be given in sublattice order and are separated by a colon.

After the component array, a sub-index digit can be specified after a semicolon. This digit must be in the range 0 to 9. The interpretation of the sub-index depends on the excess energy model used for the phase. If no semicolon and digit are given, the sub-index value is assumed to be as zero.

The excess energy parameters, e.g. the regular/subregular (binary) parameter or ternary parameters, are multiplied with two or more fractions of the constituents from the same sublattice of the solution phase. These additional constituents must be given as interacting constituents (as the following prompt).



Solution phases with sublattices can have interacting constituents in each sublattice.

## INTERACTION PARAMETER

An interaction parameter, which is used to describe the excess term of a quantity, must have two or

more constituents that interact with each other on a specified sublattice site of the given phase. It is arbitrary which of these constituents is given as the first constituent and what is given as the interacting constituents. The software always sorts the constituents (in each sublattice) in alphabetical order when the parameter name is written as a prompt (for entering its parameter value) and when the parameter is listed (using the GIBBS commands [LIST\\_PARAMETER on page 102](#) or [LIST\\_PHASE\\_DATA \(from GIBBS\) on page 103](#)). This is important for all asymmetric interaction parameters where the sign of the interaction parameter must depend on the appearance order.

Use an asterisk\* to denote that the excess interaction parameter is independent of the constituents of a specific sublattice. For example, `L (FCC_L12, AL, NI : *)` means that the interaction parameter is for the binary interaction between constituents AL and NI on the first sublattice in the FCC\_L12 solution phase, while it is independent of all constituents on the second sublattice. An interaction parameter in the list of constituents is always added to the Gibbs energy and the asterisk \* is calculated with the term of  $[1\sum y$  (specified constituents)], which implies that in an A-B binary system these `L` parameters are identical (but in higher-order systems, these are different):

- `L (phase, A, B)` is multiplied with  $X(A)*X(B)$
- `L (phase, A, *)` is multiplied with  $X(A)*(1-X(A))$
- `L (phase, B, *)` is multiplied with  $X(B)*(1-X(B))$

If you press <Enter> when you are asked for a parameter name or if you have improperly input the entire parameter name, you are asked for each of these items in the name.

## ENTER\_PARAMETER




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



Also see [About the ENTER\\_PARAMETER Command on page 95](#) for details about each of the options.

Use this command to enter TP-function(s) for a specific parameter for a phase interactively with this command. If there is already a parameter expression defined (for this parameter), that is deleted and replaced with newly entered one.

The entered TP-Function(s) for the parameter can be changed later with the command [AMEND\\_PARAMETER on page 44](#).

Syntax	ENTER_PARAMETER
Prompts	<p>PARAMETER: &lt;PARAMETER NAME&gt;</p> <p>As explained in <a href="#">About the ENTER_PARAMETER Command on page 95</a>, specify a correct and complete Parameter Name, which should contain all the necessary parts of the general form:</p> <p>&lt;IDENTIFIER&gt;(&lt;PHASE&gt;,&lt;CONSTITUENT ARRAY&gt;;&lt;DIGIT&gt;)</p> <p>If a parameter name is not acceptable or &lt;Enter&gt;, is pressed, a message displays:</p> <p>*** Error, please re-enter each part separately</p> <p>and you are prompted for input for each required part for a parameter name.</p>
Options	Description or Information
IDENTIFIER	<p>IDENTIFIER (/X/): &lt;G OR L, OR TC, OR EM, OR V0 OR VA OR VB OR VC OR VK&gt;</p> <p>If this command is used one or more times, the previous value on this prompt is set as default. Press &lt;Enter&gt; for the same type identifier or specify a new type.</p>
PHASE NAME	<p>PHASE NAME (/ABCD/): &lt;PHASE NAME&gt;</p> <p>Each parameter is valid for a specific phase only. The name of that phase must be supplied (maximum 24 characters). The name can be abbreviated.</p>
CONSTITUENT	<p>CONSTITUENT (IN SUBLATTICE # /ABC/): &lt;SPECIES NAME&gt;</p> <p>A parameter is identified by the constituents on a specified sublattice site of the given phase, the stoichiometric coefficients of which are multiplied with the parameter. The name of the constituent can be abbreviated.</p> <p> It is the species name, not the stoichiometric formula required here.</p> <p>If this command is used one or more times, the previous value on this prompt is set as default. Accept it by pressing &lt;Enter&gt; if the constituent is the same, or specify a new species name.</p>
INTERACTING CONSTITUENT	<p>For phases with several sublattices, the program asks for one constituent in each sublattice.</p> <p>INTERACTING CONSTITUENT (IN SUBLATTICE # /XYZ/): &lt;SPECIES NAME&gt;</p> <p>If this command is used one or more times, the previous value on this prompt is set as default. Press &lt;Enter&gt; to accept it if the constituent is the same, or specify a new species name.</p>

Syntax	ENTER_PARAMETER
	<p> To cancel the default value of the interacting constituent type <code>NONE</code> or the name of another constituent.</p> <p>This question is repeated until all the interested interacting constituent(s) on a specific sublattice in the phase are specified, and finally an &lt;Enter&gt; is enforced.</p>
DEGREE	<p>DEGREE /#/ : &lt;DEGREE&gt;</p> <p>Degree is model-dependent. Specify an integer number (a value from 0 through 9) as the degree of composition-dependent interaction contribution for the phase parameter. This is valid for excess energy (<code>L</code>), Curie temperature (<code>TC</code>) and Bohr magneton number (<code>BMAGN</code>), as well as for volume-related parameters (<code>V0</code>, <code>VA</code>, <code>VB</code>, <code>VC</code> or <code>VK</code>).</p> <p>For binary interaction parameters, the degree is usually the power in the Redlich-Kister expression. For ternary interaction parameters, it is usually the Hillert ternary index.</p> <p>For a standard <code>G</code> parameter for a pure component (end-member) its degree should be always 0 and this prompt should not display.</p>
PHASE PARAMETER	<p>After this prompt, the program echoes on the screen the full TP-Function of the phase parameter.</p> <p>LOW TEMPERATURE LIMIT /298.15/: &lt;LOWEST TEMPERATURE LIMIT IN K&gt;</p> <p>Specify the lowest temperature limit (in Kelvin), or the lowest-pressure limit (in Pascal but entered as a negative number), for the current TP-Function.</p> <p>FUNCTION: &lt;DEFINITION FOR A FUNCTION&gt;</p> <p>A TP-Function consists of terms in T and P.</p> <p>&amp; &lt;CONTINUATION OF THE DEFINITION FOR THE CURRENT FUNCTION&gt;</p> <p>Continuation of a TP-Function definition.</p> <p>HIGH TEMPERATURE LIMIT /6000/: &lt;HIGH TEMPERATURE LIMIT IN K&gt;</p> <p>Specify the high temperature limit (in Kelvin), or the high-pressure limit (in Pascal; only if the <i>lowest limit</i> is entered as a negative number) for the current TP-Function.</p> <p>ANY MORE RANGES /N/: &lt;Y OR N&gt;</p> <p>Enter <code>Y</code> for more function(s) or <code>N</code> to end this command.</p>

## About the ENTER\_PHASE Command

With the command *ENTER\_PHASE* on page 69, the phase name, phase-type, sublattice number, and constituents or constituent array(s) for the phase are entered into the GIBBS workspaces.

### About Phase Names

A thermochemical system must have at least one phase (which is a homogeneous part of the system with a uniform composition and structure). In the GIBBS module, any number of phases can be entered for a system and for each phase there must be a description of how its Gibbs energy varies with temperature, pressure and composition. A phase has a large amount of data connected to it, e.g. it starts with a phase name:

- It may be treated as a special phase-type;
- It may have structural information about sublattice(s), etc.,
- There must be a list of constituents (for a substitutional phase with no sublattice) or of constituent arrays (for a sublattice phase);
- There may be basic information on what kind of EXCESS\_MODEL (polynomial expression) is used to describe the binary, ternary and/or higher-order interactions between constituents;
- There may be so-called Additional contributions to the Gibbs energy of the phase from special physical phenomena, e.g. magnetic ordering, hypothetical electrostatic interaction, and so forth;
- There must exist all the parameters required for the descriptions of thermochemical properties (i.e.  $G$  terms for standard Gibbs energies, and  $L$  terms for binary, ternary or higher-order interaction excess energies) and of some special physical properties (e.g. the Curie temperature  $T_C$  and Bohr magneton number  $B_{MAGN}$  (or  $BM$ ) for magnetic ordering,  $V0$ - $VA$ - $VB$ - $VC$ - $VK$  parameters for volume contributions, Born functions for hypothetical electrostatic interaction in an aqueous solution phase) stored in connection with the phase.

### About Phase Type Code

A  $G$  phase (gaseous mixture) or an  $A$  phase (aqueous solution) is usually treated as a substitutional phase without sublattice, and that an  $L$  phase (ordinary liquid solution) is normally (but not always) modelled as a substitutional phase without sublattice, too.

The  $F$  and  $B$  phase-types are useful for ordered FCC (or HCP) and BCC solution phases handled by the so-called Four Substitutional-Sublattice Ordering Model, which always requires that the solution phase must have four sublattices for substitutional ordering and can additionally have an interstitial sublattice.

For ordered FCC or HCP phases, these four substitutional sublattices represent four corners of the regular tetrahedron on these lattices all of which are the nearest neighbours. *A Normal 4-Sublattice*

*Model* requires that all the G parameters for each of end-members with the same elements but distributed on different sites be given separately. However, as these corners are identical lattice points, the phase-type option F means that the G parameters need be given only once. The possible permutations are handled automatically. To be more clarified: An A-B binary solution phase (with the element A locates on one sublattice site and B on three sublattice sites) treated by the Normal 4-Sublattice Model has to have 4 G parameters for 4 end-members, i.e.  $G(\text{phase}, A:B:B:B)$ ,  $G(\text{phase}, B:A:B:B)$ ,  $G(\text{phase}, B:B:A:B)$  and  $G(\text{phase}, B:B:B:A)$ , because of that in the general case these G parameters can be different from each other. But for the FCC and HCP orderings, these are identical and thus all G parameters of such end-members need be given only once, and the possible permutations are then automatically handled by the GIBBS module. This significantly simplifies the usage of this model (*Four Substitutional-Sublattice Ordering Model*) in multicomponent alloys.

There are restrictions on the excess parameters allowed with the phase-type option F. You can only have excess parameters of these types:

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

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

The asterisk \* means that the interaction parameter is independent on the constituents on its corresponding sublattice. No ternary interaction parameters (i.e. with three elements on one sublattice site) are allowed. The reason for this restriction is that it would be too complicated to handle all possible permutations. In the current *Four Substitutional Sublattice Ordering Model*, the binary interaction between A and B atoms is thus independent of the constituents on the other sublattices, where there are many other parameters to model the composition-dependence of the Gibbs energy (both in the ordered and disordered parts of the phase). The model for these ordered phases are always partitioned in a disordered part (with a single substitutional sublattice) and an ordered part (with four substitutional sublattices for ordering).

For ordered BCC phases, the phase-type option B means the same thing but the situation is more complicated, as the 4-sublattice ordering phase represents an irregular tetrahedron with two pairs of sites that are next nearest neighbours. Thus, for an A-B binary solution phase (with the element A locates on two sublattice site and B on other two sublattice sites) treated by the Normal 4-Sublattice Model, the end-member described by the  $G(\text{phase}, A:A:B:B)$  term has four nearest neighbour bonds between A and B atoms, whereas the end-member described by the  $G(\text{phase}, A:B:A:B)$  term has two nearest neighbour bonds between A and B atoms and two next nearest neighbour bonds



For detailed reference visit the Crystal Lattice Structure web page  
<http://www.nrl.navy.mil/mstd/branches/6390>.

The first end-member (described by the  $G(\text{phase}, A:A:B:B)$  term) represents B2- ordering and the second (described by the  $G(\text{phase}, A:B:A:B)$  term) stands for B32-ordering. There are two permutations of the  $G(\text{phase}, A:A:B:B)$  term and four permutations of the  $G(\text{phase}, A:B:A:B)$  term, automatically conducted in the Four Substitutional-Sublattice Ordering Model. And there are also two kinds of reciprocal interaction parameters, i.e.

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



An advanced feature with the phase-type options F and B is that a composition set that represents the solution phase has a suffix (indicating that it is really as an ordered or disordered phase) that is automatically added to its phase name in some listings of equilibrium calculations (when performing either single-point or stepping or mapping calculations, and when plotting the calculated property diagrams or phase diagrams). Such suffix indications can be:

- `_L12` or `_L10` for ordered FCC
- `_A1` for disordered FCC
- `_B2`, `_B32`, `_D03` or `_L21` for ordered BCC
- `_A2` for disordered BCC
- `_D019` and `_B19` for ordered HCP
- `_A3` for disordered HCP

Solution Phase	Suffix for Disordered Phase	Suffix for Ordered Phase
FCC PHASE	PHASE_A1	PHASE_L12
		PHASE_L10
BCC PHASE	PHASE_A2	PHASE_B2
		PHASE_B32
		PHASE_D03
		PHASE_L21
HCP PHASE	PHASE_A3	PHASE_D019
		PHASE_B19

## ENTER\_PHASE



See [About the ENTER\\_PHASE Command on page 67](#) for details about the phase-type and other prompts.

With this command, the phase name, phase-type, sublattice number, and constituents or constituent array(s) for the phase are entered into the GIBBS workspaces. However, for the remaining parts of thermodynamic descriptions (i.e. thermochemical and physical parameters, excess model, and possibly additional contribution term) for the phase, the GIBBS commands [ENTER\\_PARAMETER on page 99](#) and [AMEND\\_PHASE\\_DESCRIPTION on page 52](#), should be used sequentially.

Normally, data for a system are retrieved from the preset database after the elements and species are specified. This is automatically done through [GET\\_DATA](#) on page 15. In some cases, specify a phase interactively.

Syntax	ENTER_PHASE
Options	Description and Information
PHASE NAME	<p>NAME OF PHASE: &lt;PHASE NAME&gt;</p> <p>The phase name is any string starting with a letter and containing only letters, digits or the underscore character. The phase name must be unique.</p> <p>TYPE CODE: &lt;PHASE-TYPE CODE&gt;</p> <p>The Phase-type code must be specified for the phase if it is not an ordinary solution phase. Press &lt;Enter&gt; if the phase is ordinary.</p>
PHASE-TYPE	
G	<p>Gaseous mixture phase.</p> <p><input checked="" type="checkbox"/> There may only exist one gas phase in a system.</p>
A	Aqueous solution phase.
L	Liquid solution phase but not A (aqueous) or Y (ionic liquid)
Y	Ionic liquid solution phase (that is specially treated by the Ionic Two Sublattice Liquid Model).
I	A phase with charged species but not G (gaseous), A (aqueous) or Y (ionic liquid).
F	An ordered FCC or HCP solution phase with four substitutional sublattices (additionally, such a phase can also have an interstitial sublattice).
B	An ordered BCC solution phase with four substitutional sublattices (additionally, such a phase can also have an interstitial sublattice).
SUBLATTICE NUMBER	<p>NUMBER OF SUBLATTICES /1/: &lt;SUBLATTICE NUMBER&gt;</p> <p>Phases with stoichiometric constraints usually have two or more sublattices. On each sublattice one or more species can be entered as constituents. The number of sublattices must not exceed 10. Substitutional phases with no sublattices are treated as phases with one sublattice.</p> <p>NUMBER OF SITES ON SUBLATTICE # /1/: &lt;SITE NUMBER&gt;</p> <p>For phases with sublattices, the ratio of the sites on each sublattice (donated with #) must be given. The program asks for values for all sublattices (by repeating this question for each sublattice), but these may have a common factor extracted. It is</p>


Syntax	ENTER_PHASE
	recommended to use integer numbers as sites if possible. For substitutional phases with no sublattices, this question does not show up.
CONSTITUENTS	<p>NAME OF CONSTITUENT: &lt;CONSTITUENT NAME(S)&gt;</p> <p>For each sublattice specify at least one species as constituent. Several constituents can be given consequently (on the repeated prompt) or on the same line separated by a space. This question is repeated till pressing &lt;Enter&gt; or giving a semi-colon (;), meaning that the list of constituents is terminated by (;) or an empty line.</p> <p>WILL YOU ADD CONSTITUENTS LATER /NO/: &lt;Y OR N&gt;</p> <p>For Y add other constituents to the phase by specifying new components in e.g. an ENTER_PARAMETER command. The default is N or press &lt;Enter&gt;.</p> <p>If illegal constituents are used, you get a message e.g. when parameters are entered.</p> <p>DO YOU WANT A LIST OF POSSIBLE PARAMETERS /NO/: &lt;Y OR N&gt;</p> <p>Enter Y for a list of all possible parameters up to the fifth interaction order for the entered phase.</p>

## ENTER\_SPECIES

Specify a species from the already entered elements. The stoichiometry of the species is the chemical formula of the species. For each species, its name and chemical formula must be given.



All elements are automatically entered simultaneously as species. The constituents of a phase must be species, but there is no thermochemical data associated with the species except as constituents of a phase.

Syntax	ENTER_SPECIES
Prompt	<p>SPECIES NAME: &lt;SPECIES NAME&gt;</p> <p>Enter a unique species name. This is usually its chemical formula but it can be any string which starts with a letter and contains only letters or digits. Parenthesis () and an underscore _ are permitted. The combination /- or /+ used to denote charge.</p> <p><b>Species Names Examples</b></p> <p>NaCl<sub>2</sub>, Fe<sub>2</sub>O<sub>3</sub>, FeO<sub>3/2</sub>, Fe<sub>101.5</sub>, Ca<sub>5</sub>Mg<sub>5</sub>Si<sub>103</sub>,</p> <p>Al<sub>1</sub>H<sub>101</sub>_Al(OH) , Al<sub>1</sub>H<sub>101</sub>_HALO, C<sub>2</sub>H<sub>4</sub>O<sub>3</sub>_124TRIOXOLANE, Na<sup>+</sup>, SiO<sub>4</sub><sup>-4</sup>, H<sub>1</sub><sup>+/+1</sup>, H<sub>101</sub><sup>-1</sup>, AgC<sub>2</sub>N<sub>2</sub>-1.</p> <p>The species name can be used to separate isomers with the same stoichiometry, e.g. C<sub>2</sub>H<sub>2</sub>Cl<sub>2</sub>, (CHCl)<sub>2</sub>_cis, (CHCl)<sub>2</sub>_trans, CH<sub>2</sub>_CCl<sub>2</sub>.</p>
	<p>STOICHIOMETRY /SPECIES NAME/: &lt;CHEMICAL FORMULA&gt;</p> <p>The elements in the chemical formula are normally separated by stoichiometric numbers. Neither parenthesis () nor an underscore _ is allowed in the chemical formula, while the special combination /- or /+ can be used.</p> <p>In upper case mode (see <a href="#">REINITIATE on page 83</a>), the stoichiometric number unity can be excluded only if the element symbol consists of two letters. In lower case mode, the element must be typed with the first letter in UPPER case and the second in lower, and it is thus possible to distinguish CO (carbon monoxide) from Co (cobalt) without any stoichiometry number.</p> <div>  <p>All elements in a species must be entered prior to entering the species.</p> </div>

## ENTER\_SYMBOL

In the GIBBS module, a symbol can be used to represent a numeric quantity (e.g. a *variable*), a *function*, or a *table*. The entered symbol (with a symbol name of maximum eight characters) can be used later when parameters are entered, and this is a flexible way to manipulate thermodynamic functions. Symbols are especially useful if the same function or table is used in several thermochemical parameters. A *parameter* symbol is used to assign the values of phase parameters (which are defined with the command [ENTER\\_PARAMETER on page 99](#)) to specific characterized symbols. If you want to define a constant quantity, enter it as a simple function with a constant value in all (temperature) ranges.

The symbols entered in the GIBBS module can also be listed and used in the [PARROT Commands on page 86](#) (for data optimization) where you can use the GIBBS-entered symbols (variables, functions or parameters) to define parameters that shall be optimized.



Symbols entered in the GIBBS module are not the same symbols as defined in the POLY and POST modules.





Also see [ENTER\\_SYMBOL](#) on page 195 for the POLY and POST modules.



See example 44 in the *Console Mode Examples Guide* for an example of using variables and functions.

Syntax	ENTER_SYMBOL
Prompt	<p>VARIABLE, FUNCTION, TABLE OR PARAMETER? /FUNCTION/: &lt;KEYWORD&gt;</p> <p>The <code>keyword</code> can be a variable, function, table or parameter.</p> <ul style="list-style-type: none"> <li>• <code>Variables</code> are similar to functions because these can also be expressions of state variables. It is possible to enter a variable with a new expression anytime.</li> <li>• <code>Functions</code> are expressions of state variables or other functions.</li> <li>• <code>Tables</code> are used for listing results. A table consists of a list of any number of state variables, functions or variables.</li> <li>• <code>Parameter</code> symbols are used to assign the values of phase parameters (which are defined by the command ENTER_PARAMETER) to specific characterized symbols. If the phase parameter is not defined yet, the parameter symbol is assigned zero or a symbol which is valued as zero. In this way it is easy to refer to entered phase parameters in further defining other phase parameters.</li> </ul> <p>NAME: &lt;NAME OF THE SYMBOL&gt;</p> <p>Each symbol has a unique name that must start with a letter and can have maximum 8 characters.</p> <p>The following prompts are based on the type of symbol.</p>
Variable symbol	<p>VALUE: &lt;NUMERIC VALUE OF A VARIABLE&gt;</p> <p>Only a constant numeric value, not an expression, is accepted.</p>
Function symbol	<p>Enter the lower-temperature limit, the expression, an upper-temperature limit and if there is another expression above this upper limit:</p> <p>LOW TEMPERATURE LIMIT /298.15/: &lt;LOWEST TEMPERATURE LIMIT IN K&gt;</p>

Syntax	ENTER_SYMBOL
	<p>Specify the lowest-temperature limit, below which its (first) expression is not applicable. The default lowest limit of all kinds of data is 298.15 K.</p> <p>If a negative number is given as the lowest-temperature limit, it is assumed that there are breakpoints in pressure for this function; in such a case, it is interpreted as the lowest-pressure limit (in Pascal), and the other limits in the current function are also taken as pressure limit values (in Pascal).</p> <p>The temperature/pressure limits for the functions are checked during calculations. An indicator is set if the actual temperature/pressure condition is below the lowest temperature/pressure limit or above the highest temperature/pressure limit; and in such a case, an extrapolation is conducted using the TP-FUNCTIONS valid in the nearest temperature/pressure range.</p> <p>FUNCTION: &lt;DEFINITION FOR A TP-FUNCTION&gt;</p> <p>A TP-Function consists of terms in T and P. The expression is a FORTRAN-like expression and operators +, -, *, = and ** can be used (** only with integer powers). Unary-functions LN or LOG (both for natural logarithm) and EXP (for exponential) can also be used. An expression can be continued on more than one line. A PT-function must be terminated by a semicolon (;) or an empty line. No more than 78 characters can be written on a line. If this is not sufficient space on one line, press &lt;Enter&gt; and continue on the next line. The program prompts with an ampersand &amp; when a continuation is expected.</p> <p> A function can have several temperature ranges, and a different expression (i.e. a TP-Function) for each region; if required, a single function can have up to ten different temperature ranges (and thus have up to ten different TP-Functions).</p> <p>This question is repeated if the current function has more than one expression (TPFunction) in various temperature ranges [or pressure ranges; only if the <i>lowest limit</i> is entered as a negative number]].</p> <p>&amp; &lt;CONTINUATION OF THE DEFINITION FOR THE CURRENT TP-FUNCTION&gt;</p> <p>This is for a continuation of the definition for the current TP-Function. The ampersand &amp; means that you can continue to write the function on the new line if one line is not enough for the current TP-Function. If you are finished the current TP-Function, press &lt;Enter&gt; again.</p> <p>HIGH TEMPERATURE LIMIT /6000/: &lt;HIGH TEMPERATURE LIMIT IN K&gt;</p> <p>For a TP-Function, specify the high-temperature limit, above which its current expression is not applicable. The default high-temperature limit for all kinds of data is</p>


Syntax	ENTER_SYMBOL
	<p>always 6000 K.</p> <p>This question is repeated if the function has more than one expression (TPFunction) in various temperature ranges.</p> <p> All the temperature limits for the presently-be-entered TP-Function MUST be in an increasing order; otherwise the whole function is given a single value of zero.</p> <p>If a negative number is given as the lowest-temperature limit, it is interpreted as the low-pressure limit (in Pascal), and the high-temperature limit is also taken as the high-pressure limit (in Pascal) for the current TP-Function.</p> <p>The high-temperature/pressure limit for the current applicable expression (TPFunction) is the low temperature/pressure limit for the next range if several ranges are needed to describe the temperature/pressure-dependence of this function.</p> <p>The temperature/pressure limits for the functions are checked during calculations. An indicator is set if the actual temperature/pressure condition is below the lowest temperature/pressure limit or above the highest temperature/pressure limit; and in such a case, an extrapolation is conducted using the TP-Function valid in the nearest temperature/pressure range.</p> <p>ANY MORE RANGES /N/: &lt;Y OR N&gt;</p> <p>Answer N to finish the definition of the current function. If Y the program asks for a new function valid above the last high temperature limit and below a new high temperature limit. The maximum number of temperature ranges is 10.</p> <p>Important note: Make sure that the function and its first derivatives are continuous across break points.</p>
Table symbol	<p>Specify the low and high temperature limits, temperature step and tabled value at each specified temperature:</p> <p>LOW TEMPERATURE LIMIT /298.15/: &lt;LOW TEMPERATURE LIMIT IN K&gt;</p> <p>The lowest temperature where the table has a value.</p> <p>HIGH TEMPERATURE LIMIT /6000/: &lt;HIGH TEMPERATURE LIMIT IN K&gt;</p> <p>The highest temperature where the table has a value.</p> <p>STEP IN TEMPERATURE /100/: &lt;TEMPERATURE STEP&gt;</p> <p>The step in temperature between each value in the table. This step must be constant for the whole table. If a table cannot be described with a single step it must be divided</p>

Syntax	ENTER_SYMBOL
	<p>into several tables for different temperature ranges. The upper and lower limits are truncated to give reasonable values where the table values must be specified.</p> <pre>TABLE VALUE AT  XX /YY/: &lt;TABLE VALUE&gt;</pre> <p>The value of the table at the specified temperature (xx) must be given. The default value (yy) is the last value.</p>
Parameter symbol	<p>Input the correct name of a phase parameter (including its identifier, phase name, constituent and interacting constituent(s) in various sublattices (if exist), and degree of the parameter. Most of the settings are the same as in the <a href="#">ENTER_PARAMETER on page 99</a> command or the Function symbol prompts above.</p> <pre>PARAMETER: &lt;PARAMETER NAME&gt;</pre> <p>Specify a correct and complete parameter name, which should contain all the necessary parts of the general form:</p> <pre>&lt;IDENTIFIER&gt; (&lt;PHASE&gt;, &lt;CONSTITUENT ARRAY&gt;; &lt;DIGIT&gt;)</pre> <p>If a parameter name is not acceptable or &lt;Enter&gt; is pressed, this error message displays:</p> <pre>*** ERROR, PLEASE RE-ENTER EACH PART SEPARATELY</pre> <p>The program prompts for separate input for each required part for a parameter name.</p> <pre>IDENTIFIER (/X/): &lt;G OR L, OR TC, OR BM, OR V0 OR VA OR VB OR VC OR VK&gt;</pre> <p>Specify one of these types of legal identifiers.</p> <pre>PHASE NAME (/ABCD/): &lt;PHASE NAME&gt;</pre> <p>Specify the phase name.</p> <pre>CONSTITUENT (IN SUBLATTICE # /ABC/): &lt;SPECIES NAME&gt;</pre> <p>Specify the constituent name on the specified sublattice site of the given phase.</p> <pre>INTERACTING CONSTITUENT (IN SUBLATTICE # /XYZ/): &lt;SPECIES NAME&gt;</pre> <p>Specify the interacting constituent name on the specified sublattice site of the given phase; if there is no interacting constituent, press &lt;Enter&gt;.</p> <pre>INTERACTING CONSTITUENT (IN SUBLATTICE # /XYZ/): &lt;SPECIES NAME&gt;</pre> <p>If there is more than one interacting constituent on the specified sublattice site of the given phase, specify them; otherwise press &lt;Enter&gt;.</p> <pre>DEGREE /#/: &lt;DEGREE&gt;</pre> <p>Specify an integer number (a value from 0 through 9) as the degree for the phase</p>



Syntax	ENTER_SYMBOL
	<p>parameter.</p> <p>LOW TEMPERATURE LIMIT /298.15/: &lt;LOWEST TEMPERATURE LIMIT IN K&gt;</p> <p>Specify the lowest-temperature limit (in Kelvin), or the lowest-pressure limit (in Pascal but entered as a negative number), for the current TP-Function.</p> <p>FUNCTION: &lt;DEFINITION FOR A FUNCTION&gt;</p> <p>Specify the desired TP-Function for the current temperature range (or current pressure range; only if the <i>lowest limit</i> is entered as a negative number).</p> <p>&amp; &lt;CONTINUATION OF THE DEFINITION FOR THE CURRENT TP-FUNCTION&gt;</p> <p>Specify the desired TP-Function continuation for the current temperature range (or current pressure range; only if the lowest limit is entered as a negative number).</p> <p>HIGH TEMPERATURE LIMIT /6000/: &lt;HIGH TEMPERATURE LIMIT IN K&gt;</p> <p>Specify the high-temperature limit (in Kelvin), or the high-pressure limit (in Pascal; only if the lowest limit is entered as a negative number) for the current TP Function.</p> <p>ANY MORE RANGES /N/: &lt;Y OR N&gt;</p>

## LIST\_CONSTITUENT

Syntax	LIST_CONSTITUENT
	List all the constitutions (as site-fractions) for all the phases in the defined system.
	 This is mainly for software managers. There are no commands in the GIBBS monitor to set the constitution.

## LIST\_DATA

All data for the current system that is defined (retrieved from database in the DATA module, or directly entered in the GIBBS module) within the current GIBBS workspace is written in a readable manner on the output file. If no output file is specified, the data display on screen.

The output data consists of a list of all elements and their data followed by a list of all phases and the data associated with each phase. The thermochemical parameters listed for each phase are always in SI units.



For encrypted commercial databases you may not be able to use this command to list any retrieved data. However, it can be used to list some basic definitions (such as phase models and phase-constituents) retrieved from an encrypted database, as well as all the references related to original assessments (but not thermodynamic parameters) for the currently-defined system.

Syntax	LIST_DATA
Prompts	<p>OUTPUT TO SCREEN OR FILE /SCREEN/: &lt;FILE NAME&gt;</p> <p>Specify the name of a file in which the data shall be written in a readable manner. The default value is the screen (by pressing &lt;Enter&gt;).</p>
	<p>OPTIONS?: &lt;OPTION(S)&gt;</p> <p>Choose one or several of these options for output:</p> <ul style="list-style-type: none"> <li>• <b>N</b> the output is written as a user database format.</li> <li>• <b>P</b> the output is written as a macro file for future input. This is useful for creating *SETUP files for data assessments.</li> <li>• <b>S</b> the symbols are suppressed.</li> <li>• <b>R</b> the references for the parameters are listed (only for some databases in which references are available)</li> <li>• <b>L</b> the output is written suitable for a LaTeX preprocessor.</li> </ul>

## LIST\_PARAMETER


This command is for both the GIBBS and PARROT modules.

List the TP-function(s) of a specific parameter for a phase. You must supply the name of the phase parameter:

THE PARAMETER NAME: <IDENTIFIER>(<PHASE>,<CONSTITUENT ARRAY>;<DIGIT>)



For encrypted commercial databases, you may not be able to use this command to list any retrieved parameter.

Syntax	LIST_PARAMETER
Prompts	<p>PARAMETER: &lt;PARAMETER NAME&gt;</p> <p>Specify a correct and complete parameter name, which should contain all the necessary parts of the general form: &lt;identifier&gt;(&lt;phase&gt;,&lt;constituent array&gt;;&lt;digit&gt;)</p> <p> See <a href="#">About the ENTER_PARAMETER Command on page 95</a> to learn how to define the Parameter Name.</p> <p>If a parameter name is not acceptable or &lt;Enter&gt; is pressed, an error message displays:</p> <pre>*** Error, please re-enter each part separately</pre> <p>The program prompts for separate input for each required part for a parameter name.</p>
	<p>IDENTIFIER (/X/): &lt;G OR L, OR TC, OR BM, OR V0 OR VA OR VB OR VC OR VK&gt;</p> <p>Specify one of these types of legal identifiers.</p>
	<p>PHASE NAME (/ABCD/): &lt;PHASE NAME&gt;</p> <p>Specify the phase name.</p>
	<p>CONSTITUENT (IN SUBLATTICE # /ABC/): &lt;SPECIES NAME&gt;</p> <p>Specify the constituent name on the specified sublattice site of the given phase.</p>
	<p>INTERACTING CONSTITUENT (IN SUBLATTICE # /XYZ/): &lt;SPECIES NAME&gt;</p> <p>Specify the interacting constituent name on the specified sublattice site of the given phase; if there is no interacting constituent, press &lt;Enter&gt;.</p>
	<p>INTERACTING CONSTITUENT (IN SUBLATTICE # /XYZ/): &lt;SPECIES NAME&gt;</p> <p>If there is more than one interacting constituent on the specified sublattice site of the given phase, specify them; otherwise press &lt;Enter&gt;.</p>
	<p>DEGREE /#/ : &lt;DEGREE&gt;</p> <p>Specify a numerical number as the degree for the phase parameter.</p>

## LIST\_PHASE\_DATA

All data for a specific phase are written in a readable manner on screen. The thermochemical parameters listed for the phase are always in SI units.



For encrypted commercial databases you may not be able to use this command to list any phase data. However, this command can be used for listing some basic definitions (such as phase model and phase-constituents) for the specified phase, as well as all the references related to original assessments (but not thermodynamic parameters) for the currently-defined system.

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

## LIST\_STATUS

Syntax	LIST_STATUS
	<p>For the GIBBS module, list the entered elements, phases and species with the status word. The command is included for system managers.</p> <p> Each element, species, phase and symbol has a set of status bits. The values of these bits are listed with this command.</p> <p>The bits are listed as hexadecimal, i.e. four bits are written as a hexadecimal number. Two hexadecimal numbers make a byte. In hexadecimal, 0 to 9 mean normal digits. A to F means values 10 to 15. The number <code>E4000000</code> has thus bit 1, 2, 3 and 6 equal to one. The bits are numbered starting with 1 for the most significant (leftmost) bit.</p>

### Element Status Word

Set the element status word (*Bit. Meaning*) if:

1. Element cannot be deleted (only vacancy and electron)
2. Suspended (inclusive OR of bit 3 and 4)
3. Explicitly suspended
4. Implicitly suspended (cannot occur for an element)

### Species Status Word

Set species status word (*Bit. Meaning*) if:

1. Species record for an element (each element has a species record)
2. Suspended (inclusive OR of bit 3 and 4)

3. Explicitly suspended
4. Implicitly suspended (e.g. if a species element is suspended)
5. Charged (inclusive OR of bit 6 and 7)
6. Negative charge
7. Positive charge
8. Vacancy
9. Component (by default the elements are the components)

### Phase Status Word

Set phase status word (*Bit. Meaning*) if:

1. Ideal (no sublattices and no excess parameters)
2. Suspended (inclusive OR of bit 3 and 4)
3. Explicitly suspended
4. Implicitly suspended (e.g. if all constituents suspended)
5. Gas phase
6. Liquid phase
7. Solution phase
8. Only one constituent (in each sublattice)
9. Ions (inclusive OR of bit 10 and 12)
10. New ionic liquid model (charge balance handled internally)
11. Constituents cannot be added
12. External charge balance needed
13. Aqueous model
14. Charged species (ions)
15. Dilute entropy
16. Last calculation exceeded temperature range for any parameter
17. Kapoor-Frohberg-Gaye cell model
18. Turbo calculation used
19. Turbo calculation impossible
20. Turbo calculation illegal

21. Phase is not ideal
22. Current site fractions saved
23. This phase is the ordered part
24. This phase is the disordered part (bit 2 and 3 also set)
25. Shadow phase with diffusion data
26. Error in ionic model
27. Sometimes
28. CVM-SRO (short-range ordering) entropy expression
29. CVM initialization is made
30. Used to test quasi-chemical ordering model
31. Major constituents check even if no miscibility gap (ordering)
32. Hoch-Arpschhofen model

### Symbol Status Word

Set symbol status word (*Bit meaning*) if:

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

## LIST\_SYMBOL

List the symbols available in the current GIBBS workspace, which are defined (retrieved from database in the DATA module, or directly entered in the GIBBS module) and used in TP-functions for the entered model parameters for various phases in the defined system.



For encrypted commercial databases you may not be able to use this command to list any retrieved symbol.

Syntax	LIST_SYMBOL
Prompts	<p>NAME: &lt;SYMBOL NAME&gt;</p> <p>Specify a symbol name (either as the full name of a defined symbol, or as the first few common characters of several symbols which have names starting with such common characters).</p> <p><input checked="" type="checkbox"/> Only those symbols that match this name are listed.</p> <p>Or press &lt;Enter&gt; for a list of all the symbols defined (retrieved from database in the DATA module, or directly entered in the GIBBS module) for the current system, which are available in the current GIBBS workspace.</p>
	<p>OUTPUT TO SCREEN OR FILE /SCREEN/: &lt;FILE NAME&gt;</p> <p>Specify the name of a simple-textual file in which the entered symbols shall be written in a readable manner (such a basic textual file can later on be opened and edited by any text editor). The default value is the screen (by pressing &lt;Enter&gt;).</p>

## READ\_GES\_WORKSPACE

The data area saved onto a \*.GES5 file with [SAVE\\_GES\\_WORKSPACE](#) on the next page is read back into the GIBBS workspace.

Syntax	READ_GES_WORKSPACE
	<p>Enter a <b>File name</b> and specify the working directory where to save the file in the <b>Look in</b> field. Normally the default file-type in the <b>Files of type</b> field is the correct one for the GIBBS workspace format (i.e. *.GES5 file).</p> <p><input checked="" type="checkbox"/> The saved *.GES5 files are unique for each CPU type, and therefore a *.GES5 file saved on one CPU type cannot be read and used on another CPU type.</p>

## REINITIATE


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

Syntax	REINITIATE
Prompts	<p>UPPER CASE ONLY /Y/: &lt;Y OR N&gt;</p> <p>The name of elements and species can be either in only UPPER case (by typing Y or pressing &lt;Enter&gt;), or the elements with two letter names have the first letter in Upper and the second in lower case (by typing N).</p> <p><input checked="" type="checkbox"/> In upper case mode all input in lower case is automatically converted to upper case.</p>
	<p>LOWER TEMPERATURE LIMIT /298.15/: &lt;LOWEST T IN K&gt;</p> <p>This value is used as the lower temperature limit when data are entered interactively.</p>
	<p>UPPER TEMPERATURE LIMIT /6000/: &lt;HIGHEST T IN K&gt;</p> <p>This value is used as the upper temperature limit when data are entered interactively.</p>
	<p>DEFAULT ELEMENT REFERENCE STATE SYMBOL INDEX /1/: &lt;1 OR 2 OR 3&gt;</p> <p>Specify a proper index for the default listing parameters (symbol), or press &lt;Enter&gt; to accept the preset index 1.</p> <p>The <i>index</i> is for defining the symbol printed in listings of parameters. The symbol can be:</p> <ul style="list-style-type: none"> <li>• G: the data are referred to Gibbs energy at a variable temperature (also called <i>Lattice Stability</i>).</li> <li>• H<sub>298</sub>: the data are referred to the enthalpy of the element at 298.15 K and 1 bar.</li> <li>• H<sub>0</sub> is the same as H<sub>298</sub> but at the temperature 0 K.</li> </ul> <p><input checked="" type="checkbox"/> The index only changes the symbol, not any value. Normally the index is set correctly by the database. Only when manually entering data must you set the index to get the correct symbol. Set the index value to 0 to get the symbol G, to 1 to get the symbol H<sub>298</sub> and to 2 to get H<sub>0</sub>.</p>

## SAVE\_GES\_WORKSPACE

The data area used by the GIBBS workspace can be saved on a file (with a default extension GES5 under MS-Windows, or ges5 under Linux). The default file name is RESULT.GES5 or equal to the one used in a previous [READ\\_GES\\_WORKSPACE](#) on the [previous page](#) command.



Syntax	SAVE_GES_WORKSPACE
	<p>Enter a <b>File name</b> and specify the working directory where to save the file in the <b>Save in</b> field. Normally the default file-type in the <b>Files of type</b> field is the correct one for the GIBBS workspace format (i.e. *.GES5 file).</p> <p> The output is unformatted and cannot be printed.</p>

## SET\_R\_AND\_P\_NORM

The value of the gas constant (R) is used to define the energy units that are used for input of data. On output, all data are in SI units. The value of the pressure 1 atm is used to interpret values of the pressure given by application programs.

Syntax	SET_R_AND_P_NORM
Prompts	<p>VALUE OF GAS CONSTANT IN YOUR ENERGY UNITS /8.31451/: &lt;NEW VALUE&gt;</p> <p>The default value of the gas constant is in SI units (i.e. 8.31451). If you change this value, it only affects the interpretation of energy data given interactively from the terminal, e.g. if the value is set to 1.98717 you can give values in Calories.</p>
	<p>VALUE OF ONE BAR IN YOUR PRESURE UNITS /100000/: &lt;NEW VALUE&gt;</p> <p>The value of the pressure given in application programs is divided by this value and then multiplied with the value of one bar expressed in Pascal before it is used inside the GIBBS module.</p>

## PARROT Commands

In this section:

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<i>AMEND_PARAMETER</i> .....	88
<i>AMEND_SYMBOL</i> .....	90
<i>COMPILE_EXPERIMENTS</i> .....	92
<i>CONTINUE_OPTIMIZATION</i> .....	94
<i>CREATE_NEW_STORE_FILE</i> .....	94
<i>EDIT_EXPERIMENTS</i> .....	95
<i>About the ENTER_PARAMETER Command</i> .....	95
<i>ENTER_PARAMETER</i> .....	99
<i>LIST_ALL_VARIABLES</i> .....	101
<i>LIST_CONDITIONS</i> .....	102
<i>LIST_PARAMETER</i> .....	102
<i>LIST_PHASE_DATA (from GIBBS)</i> .....	103
<i>LIST_RESULT</i> .....	104
<i>LIST_STORE_FILE</i> .....	108
<i>LIST_SYMBOL_IN_GES</i> .....	108
<i>OPTIMIZE_VARIABLES</i> .....	109
<i>READ_PARROT_WORKSPACES</i> .....	109
<i>RECOVER_VARIABLES</i> .....	110
<i>REINITIATE</i> .....	110
<i>RESCALE_VARIABLES</i> .....	110
<i>SAVE_PARROT_WORKSPACES</i> .....	111
<i>SET_ALTERNATE_MODE</i> .....	111
<i>SET_EXTERNAL_PARAMETER</i> .....	111
<i>SET_FIX_VARIABLE</i> .....	112
<i>SET_OPTIMIZING_CONDITION</i> .....	113

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<i>SET_OPTIMIZING_VARIABLE</i> .....	<a href="#">114</a>
<i>SET_OUTPUT_LEVELS</i> .....	<a href="#">115</a>
<i>SET_SCALED_VARIABLE</i> .....	<a href="#">115</a>
<i>SET_STORE_FILE</i> .....	<a href="#">116</a>

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## AMEND\_PARAMETER


Interactively modify the TP-function(s) for a specific parameter for a phase with this command. This is useful in order to correct typing errors because the old function is made available for interactive editing on the terminal.



This AMEND\_PARAMETER command is for the PARROT module. There is also a GES module command with the same name ([AMEND\\_PARAMETER on page 44](#)).

Syntax	AMEND_PARAMETER
Prompts	<p>PARAMETER: &lt;PARAMETER NAME&gt;</p> <p>Specify a correct parameter name. If a parameter name is not acceptable or &lt;Enter&gt; is pressed, the error message displays:</p> <pre>*** ERROR, PLEASE RE-ENTER EACH PART SEPARATELY</pre> <p>The program prompts for separate input for each part for a parameter name.</p>
	<p>IDENTIFIER (/X/): &lt;G OR L, OR TC, OR BM, OR V0 OR VA OR VB OR VC OR VK&gt;</p> <p>Specify one of these types of legal identifiers (see <a href="#">ENTER_PARAMETER on page 99</a>).</p>
	<p>PHASE NAME (/ABCD/): &lt;PHASE NAME&gt;</p> <p>Specify the phase name.</p>
	<p>CONSTITUENT (IN SUBLATTICE # /ABC/): &lt;SPECIES NAME&gt;</p> <p>Specify the constituent name.</p>
	<p>INTERACTING CONSTITUENT (IN SUBLATTICE # /XYZ/): &lt;SPECIES NAME&gt;</p> <p>Specify the interacting constituent name; if there is no interacting constituent, press &lt;Enter&gt;.</p>
	<p>INTERACTING CONSTITUENT (IN SUBLATTICE # /XYZ/): &lt;SPECIES NAME&gt;</p> <p>If there is more than one interacting constituent, specify these; otherwise press &lt;Enter&gt;.</p>
	<p>DEGREE /#/ : &lt;DEGREE&gt;</p> <p>Specify a numerical number as the degree of the phase parameter.</p>
	<p>After the parameter name is specified correctly, the program lists its current definition (either preset in database or defined by the ENTER_PARAMETER command), such as:</p> <pre>L (PHASE2,AL,MG;1)= 298.15&lt;T&lt;2000.00: +5000 2000.00&lt;T&lt;4500.00: +4500</pre>

Syntax	AMEND_PARAMETER
	<pre>4500.00&lt;T&lt;6000.00: +4000</pre> <p>You are prompted to change the parameter definition:</p> <pre>DO YOU WANT TO CHANGE THE NUMBER OF RANGES /NO/: &lt;Y OR N&gt;</pre> <p>To change the number of ranges for the chosen function, or change some of the temperature limits in the definition, by typing <b>Y</b> you have to retype both the low/high temperature limits and functions</p> <p>If you do not want to change the number of ranges but want to change the function(s) in one or more ranges, press &lt;Enter&gt; to accept the default <b>N</b> the whole definition of the chosen parameter in all ranges (if any) is listed such as:</p> <pre>DIFFERENT FUNCTIONS IN THESE RANGES 298.15&lt;T&lt;2000.00 2000.00&lt;T&lt;4500.00 4500.00&lt;T&lt;6000.00</pre> <p>This message prompts:</p> <pre>DO YOU WANT TO CHANGE RANGE LIMITS /NO/: &lt;Y OR N&gt;</pre> <p>If there is more than one range, this question is prompted. Press &lt;Enter&gt;.</p>
	<pre>RANGE NUMBER (0 TO EXIT) /0/: &lt;RANGE NUMBER&gt;</pre> <p>If the function of a parameter is different in two or more temperature ranges, you must specify the range of the function of which you want to amend. Or press &lt;Enter&gt; or type <b>0</b> to exit this command without making any change.</p>
	<pre>FUNCTION</pre> <p>The previous function is available for editing. The editing is performed within the general subroutine <code>FOOLED</code>, as described in <a href="#">AMEND_SYMBOL on the next page</a>. This routine prompts as follows:</p> <pre>1:+:&gt;</pre> <p>The prompt consists of the current position in the string and the character at that position between colons, (::).</p> <h3>Commands</h3> <p>These commands can be given:</p> <ul style="list-style-type: none"> <li>• Help: <b>?</b></li> <li>• Move CP to last or first character: <b>&lt;+/-&gt; A</b></li> </ul>

Syntax	AMEND_PARAMETER
	<ul style="list-style-type: none"> <li>• Delete characters from CP: &lt;+-#characters&gt; D</li> <li>• Exit: E</li> <li>• Find: &lt;#occurrences&gt; F&lt;string&gt;@</li> <li>• Insert: I&lt;string&gt;@</li> <li>• Move: &lt;+-#positions&gt; M</li> <li>• Restore string: R</li> <li>• Substitute: S&lt;OLD&gt;@&lt;NEW&gt;@</li> <li>• Type string: T</li> </ul> <p>where CP denotes the current position in string, # means number of, @ is a terminator of an input or search string.</p> <p> When the string is typed the character at the current position is replaced by an underscore _.</p> <p>To finish the editing of the current function, type E.</p>
	<p>RANGE NUMBER (0 TO EXIT) /0/: &lt;RANGE NUMBER&gt;</p> <p>Give a range number to edit that function, or press &lt;Enter&gt; or type 0 to exit this command.</p>

## AMEND\_SYMBOL

In the GIBBS and PARROT modules, interactively calculate the current values of a function or table (predefined by the switched database or previously entered with [ENTER\\_SYMBOL](#) on page 72) at the current temperature and pressure condition, and also possible to modify the definitions of variables or functions.




The current values of the temperature and pressure used to calculate the functions or tables are the ones listed with [LIST\\_STATUS](#) on page 80. There is no way to change the current temperature and pressure values interactively.

To modify the definitions of entered symbols (variable, functions or parameters), the performance of this command is slightly different one from another, as described below:

- For variables, the values can be changed.
- For functions the low and high temperature limits in various ranges (if any), as well the expressions, can be changed.
- For parameters the low and high temperature limits in various ranges (if any), as well the expressions, can be changed.

Syntax	AMEND_SYMBOL
Prompts	<p>NAME: &lt;SYMBOL NAME&gt;</p> <p>Specify the name of an entered symbol.</p> <p>For tables and functions (or parameters which are treated as functions after these are entered by the ENTER_SYMBOL command with the <code>Parameter</code> keyword, but not by the ENTER_PARAMETER command), after the symbol name is specified here, the program automatically calculates the values under the current temperature and pressure conditions, and lists the current values, such as:</p> <pre>FUNCTION VALUE  2.52500000E+01 TABLE VALUE    1.56000000E+02</pre> <p>For variables and functions (or parameters), there are additional prompts and depend on the symbol type.</p>
	<p>For a variable, its current value is displayed, and you can change it to a new value:</p> <pre>VALUE /CURRENT VALUE/: &lt;NEW VALUE&gt;</pre> <p>For a function (or a parameter entered as a symbol):</p> <pre>DO YOU WANT TO CHANGE THE NUMBER OF RANGES /NO/: &lt;Y OR N&gt;</pre> <p>To change the number of ranges for the function, or change some of the temperature limits in the definition, For <code>Y</code>, you must retype both the low/high temperature limits and functions (see all the remaining details in the ENTER_SYMBOL command.</p> <p>If you do not want to change it, press &lt;Enter&gt; to accept the default. The definition of the chosen function in all ranges (if any) is listed, for example:</p> <pre>DIFFERENT FUNCTIONS IN THESE RANGES 298.15&lt;T&lt;2000.00 2000.00&lt;T&lt;4500.00 4500.00&lt;T&lt;6000.00</pre> <p>and this message displays:</p> <pre>Do you want to change range limits /no/: &lt;y or n&gt;</pre> <p>If a function is different in two or more temperature ranges, you must specify the range of</p>

Syntax	AMEND_SYMBOL
	the function of which you want to amend. Or press <Enter> or type 0 to exit this command without making any change.
	<p>RANGE NUMBER (0 TO EXIT) /0/: &lt;RANGE NUMBER&gt;</p> <p>FUNCTION:</p> <p>The previous function is available for editing. The editing is performed within the general subroutine FOOLED. This routine prompts as follows:</p> <p>1:+:&gt;</p> <p>The prompt consists of the current position in the string and the character at that position between colons (::).</p> <p><b>Commands</b></p> <p>These commands can be given:</p> <ul style="list-style-type: none"> <li>• Help: ?</li> <li>• Move CP to last or first character: &lt;+/-&gt; A</li> <li>• Delete characters from CP: &lt;+ -#characters&gt; D</li> <li>• Exit: E</li> <li>• Find: &lt;#occurrences&gt; F&lt;string&gt;@</li> <li>• Insert: I&lt;string&gt;@</li> <li>• Move: &lt;+ -#positions&gt; M</li> <li>• Restore string: R</li> <li>• Substitute: S&lt;OLD&gt;@&lt;NEW&gt;@</li> <li>• Type string: T</li> </ul> <p>where CP denotes the current position in the string, # means number of, @ is a terminator of an input or search string.</p> <p> When the string is typed the character at the current position is replaced by an underscore _. To finish the editing of the current function, type E at the prompt.</p>

## COMPILE\_EXPERIMENTS

The descriptions of the experimental equilibria saved on a textual \*.POP file, given as commands in the POLY and ED\_EXP syntax, is compiled by this command into the PARROT structured data, i.e. stored into



the current work \*.PAR file which is created with [CREATE\\_NEW\\_STORE\\_FILE](#) on the next page, set by [SET\\_STORE\\_FILE](#) on page 116, or opened with [READ\\_PARROT\\_WORKSPACES](#) on page 109, all done before `COMPILE_EXPERIMENTS`.

This command also lists the compilation details on screen or onto a listing file (\*.TXT).



If a syntax error in the commands is detected, the compilation is terminated. You need to correct the error in the \*.POP file (using a textual editor) and recompile it with the \*.PAR work (store) file.

After a successful compilation, the program translates all the experimental data points in the \*.POP file into a graphical experimental data file (\*.EXP) in the DATAPLOT syntax, which can be further edited and used as a graphical experimental data file (\*.EXP) for the purposes of imposing onto calculated/plotted phase diagrams and/or property diagrams for comparisons during the assessment process.



Also see the *DATPLOT User Guide* included with this documentation set.

Syntax	COMPILE_EXPERIMENTS
	A window displays to open the original experimental data file (*.POP). Enter a <b>*.POP File name</b> box, and specify the working directory in the <b>Look in</b> box. Normally the default file-type in the <b>Files of type</b> field is the correct one for the experimental data format (i.e. *.POP file). Click <b>Open</b> or <b>Cancel</b> button as applicable.
Prompts	<p>OUTPUT TO SCREEN OR FILE /SCREEN/: &lt;*.POP FILE NAME&gt;</p> <p>A list of the source code in the *.POP file and error messages during compilation is written on screen (by pressing &lt;Enter&gt;) or on a list *.TXT file under a specific file name which can later on be opened and edited by any basic textual editor.</p>
	<p>INITIATE STORE FILE /Y/: &lt;Y OR N&gt;</p> <p>After a successful compilation, the data in the POLY3 workspace is stored as a new block of equilibria on the current work (store) file. If you specify that the store file should be initiated before compilation (Y), only the compiled block is stored on the current work file (consequently, the *.PAR file is updated). If a negative answer (N) is chosen here, the current work file is not changed.</p> <p>A window displays to generate/store the graphical experimental data file (*.EXP) in the DATAPLOT syntax. Enter a *.EXP file name in the <b>File name</b> field and specify the working directory when opening the *.EXP file in the <b>Look in</b> field. Normally the default file type in the <b>Files of type</b> field is the correct one for the graphical experimental data format (i.e. *.EXP file). Click <b>Open</b> or <b>Cancel</b> as applicable.</p>

## CONTINUE\_OPTIMIZATION

This command continues the optimization using the same Hessian matrix.



In some cases it is not possible to attempt continuation. For example, if the optimization has already converged or if the optimizing parameters or the set of experimental equilibria used in the current optimization runs are changed. The program gives a warning message if you try to continue when you make these changes.

Syntax	CONTINUE_OPTIMIZATION
Prompts	<p>ARE YOU SURE? /N/: &lt;N OR Y&gt;</p> <p>Prior to this question, a message displays to confirm if it is OK to continue:</p> <p>It is safe to CONTINUE only after TOO MANY ITERATIONS and no change in variables and experiments ...</p> <p>You can accept the default (N) in order to cancel this special attempt.</p>
	<p>NUMBER OF ITERATIONS /N/: &lt;INTEGRAL NUMBER OF ITERATION&gt;</p> <p>Specify an integral number for the optimization iteration. The specified iteration number is shown as the default number. The PARROT program tries this exact number of different sets of values of the optimizing variables without stopping the optimization even it would have converged earlier or should give up earlier.</p>

## CREATE\_NEW\_STORE\_FILE



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

Create a binary file to be used as a *work file* (also called *store file*) before any optimization can be done. The workspace used by the GIBBS, POLY and PARROT modules is stored automatically on the work file but not any experimental information. The binary work file has a default extension of `PAR` under MS-Windows or `par` under Linux/UNIX.

A work file that is created at a previous run can be used in the PARROT module with the other command SET-STORE-FILE.

Syntax	CREATE_NEW_STORE_FILE
Prompt	<p>&lt;*.par file name&gt;</p> <p>A <b>Save</b> window displays. Enter a <b>File name</b> and specify the working directory in the <b>Save in</b> field. Normally the default file-type in the <b>Files of type</b> field is the correct one for the PARROT workspace format (i.e. PAR file). Click <b>Save</b> or <b>Cancel</b> as applicable.</p>

## EDIT\_EXPERIMENTS

Initialise and make available the sub-module for editing experimental equilibria, i.e. the ED\_EXP module. All experimental equilibria compiled from the \*.POP file can be accessed in the ED\_EXP module.

The ED\_EXP module is similar to the normal POLY module, but some commands are special and some POLY commands are not available. In the ED\_EXP module, you can calculate each equilibrium separately or together, provide start values for equilibria which failed to converge, set weights, and modify the values of experiments or conditions.



Also see [Running the EDIT\\_EXPERIMENTS Command on page 23](#).

Syntax	EDIT_EXPERIMENTS
	You are now in this submodule and can start using the commands.

## About the ENTER\_PARAMETER Command



For the PARROT Module, this command is the same and is described here. Also see [ENTER\\_PARAMETER on page 99](#) for the command details.

In the descriptions of the standard thermochemical properties and special physical properties for a phase, there are a number of parameters which may depend on the temperature and pressure. The expressions for these parameters can be given in a free form as a sum of terms with powers of T and P and may also include the natural logarithm and exponential function. This type of expression is called *TP-functions*. Identical parameters (in terms of parameter-names) are stored only once in the GIBBS workspaces.

The composition-dependence of the Gibbs energy is described in the GIBBS module by the internal data structure, which is created when the phase is entered (see [GIBBS\\_ENERGY\\_SYSTEM Commands on page 42](#)). The Gibbs energy of a phase is always referred to one formula unit of the phase, i.e. the amount derived from the number of sites (i.e. the stoichiometric coefficient) for each sublattice. If vacancy is a constituent of a sublattice, the amount of matter per formula unit of the phase may vary with composition.

## Defining the Parameter

A valid parameter should have the general form of:

```
<identifier>(<phase>, <constituent array>; <digit>) <xxx> <expression> <yyy> <keyword  
Y or N> <zzz> !
```

The identifier must be followed by an opening parenthesis, a phase name, a comma and a constituent array. Optionally, the constituent array can be followed by a semicolon and a digit. The parameter name is terminated by a closing parenthesis. The parameter form is defined as:

- `<identifier>` is the parameter type;
- `<phase>` is the phase name (maximum 24 characters);
- `<constituent array>` is the specific constituent array in the phase;
- `<digit>` is the degree of composition-dependent interaction contribution (an integer number from 0 through 9), that is only for excess energy (L), Curie temperature (TC) and Bohr magneton number (BMAGN), as well as for volume-related parameters (V0 or VA or VB or VC or VK); if it is valued as zero, or if it is for the standard Gibbs energy (G) for which the degree is always zero, it can be omitted;
- `<expression>` is the mathematical relation to describe the parameter;
- `<xxx>` and `<yyy>` are the low and high temperature limits respectively for the applicable temperature range of the parameter expression;
- `<keyword Y or N>` is the indicator on if there is continuation for the parameter expression or not;
- `<zzz>` is the reference index/number for the assessment of this parameter;
- The exclamation point ! is used to indicate that the current parameter definition is ended.

## PARAMETER NAME

The GES parameter name has a general form of:

```
<identifier>(<phase>,<constituent array>;<digit>)
```

Examples of parameter names:

- `G(GAS,C1O2)` : The Gibbs energy of formation of a CO<sub>2</sub> molecule in gas.
- `G(FCC,Fe:VA)` : The Gibbs energy of formation of fcc Fe with interstitials.
- `L(LIQ,Fe,Cr;0)` : The regular solution parameter for Fe and Cr in liquid.
- `L(LIQ,Fe,Cr;1)` : The sub-regular solution parameter.
- `TC(BCC,Fe:Va)` : The Curie temperature of bcc Fe.
- `BMAGN(BCC,Fe:Va)` : The Bohr magneton number parameter of bcc Fe.

The parameter name consists of several parts. The first is a type-identifier and these can be used:

- **G**: Standard energy parameter (Gibbs energy of formation) or for interaction

parameters;

- **L**: Excess energy parameter (Gibbs energy of interaction) always used for interaction parameters;
- **TC**: Curie temperature for magnetic ordering;
- **BMAGN** or **BM**: Bohr magneton number for magnetic ordering (or Born function  $\omega_{Pr,Tr}$  for aqueous solute species).
- **VO**: Molar volume at 298.15 K and 1 bar (a numeric value only);
- **VA**: Integrated thermal expansivity;  $\int_{298.15}^T \alpha(T) dT$   $\int_{298.15}^T \alpha(T) dT$
- **VB**: Bulk modulus at 1 bar;
- **VC**: Isothermal compressibility;
- **VK**: High-pressure fitting parameter.



When necessary quantities as **H** (enthalpy), **S** (entropy), **V** (Volume), **F** (Helmholtz energy), etc., can be calculated from the Gibbs energy.

## PHASE NAME

Specifying the `PHASE NAME` in uppercase is recommended; however, if you prefer to write it as a mixture of uppercase and lowercase, it automatically converts all lowercase to uppercase, as the GIBBS module only recognises uppercase phase names. It is important that if a phase bears a legal phase-type (among G, A, Y, L, I, F and B) in its phase definition (already by the `PHASE` keyword; such as `GAS:G`, `LIQUID:L`, `SLAG:L`, `IONIC-LIQ:Y`, `SPINEL:I`, `FCC_L12:F`, `HCP_D021:F`, `BCC_B2:B`, `AQUEOUS:A`), such a valid phase-type code should not be attached to the phase name when `ENTER_PARAMETER` is executed.

## CONSTITUENT ARRAY

The constituent array consists of a list of constituent names. Interaction parameters have two or more constituents from the same sublattice separated by a comma. If the phase has sublattices, at least one constituent in each sublattice must be specified. The constituents in different sublattices must be given in sublattice order and are separated by a colon.

After the component array, a sub-index digit can be specified after a semicolon. This digit must be in the range 0 to 9. The interpretation of the sub-index depends on the excess energy model used for the phase. If no semicolon and digit are given, the sub-index value is assumed to be as zero.

The excess energy parameters, e.g. the regular/subregular (binary) parameter or ternary parameters, are multiplied with two or more fractions of the constituents from the same sublattice of the solution phase. These additional constituents must be given as interacting constituents (as the following prompt).



Solution phases with sublattices can have interacting constituents in each sublattice.

## INTERACTION PARAMETER

An interaction parameter, which is used to describe the excess term of a quantity, must have two or more constituents that interact with each other on a specified sublattice site of the given phase. It is arbitrary which of these constituents is given as the first constituent and what is given as the interacting constituents. The software always sorts the constituents (in each sublattice) in alphabetical order when the parameter name is written as a prompt (for entering its parameter value) and when the parameter is listed (using the GIBBS commands [LIST\\_PARAMETER on page 102](#) or [LIST\\_PHASE\\_DATA \(from GIBBS\) on page 103](#)). This is important for all asymmetric interaction parameters where the sign of the interaction parameter must depend on the appearance order.

Use an asterisk\* to denote that the excess interaction parameter is independent of the constituents of a specific sublattice. For example, `L (FCC_L12, AL, NI : *)` means that the interaction parameter is for the binary interaction between constituents AL and NI on the first sublattice in the `FCC_L12` solution phase, while it is independent of all constituents on the second sublattice. An interaction parameter in the list of constituents is always added to the Gibbs energy and the asterisk \* is calculated with the term of  $[1\sum y(\text{specified constituents})]$ , which implies that in an A-B binary system these `L` parameters are identical (but in higher-order systems, these are different):

- `L (phase, A, B)` is multiplied with  $X(A) \cdot X(B)$

- $L(\text{phase}, A, *)$  is multiplied with  $X(A) \cdot (1 - X(A))$
- $L(\text{phase}, B, *)$  is multiplied with  $X(B) \cdot (1 - X(B))$

If you press <Enter> when you are asked for a parameter name or if you have improperly input the entire parameter name, you are asked for each of these items in the name.

## ENTER\_PARAMETER



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



Also see [About the ENTER\\_PARAMETER Command on page 95](#) for details about each of the options.

Use this command to enter TP-function(s) for a specific parameter for a phase interactively with this command. If there is already a parameter expression defined (for this parameter), that is deleted and replaced with newly entered one.

The entered TP-Function(s) for the parameter can be changed later with the command [AMEND\\_PARAMETER](#) on page 44.

Syntax	ENTER_PARAMETER
Prompts	<p>PARAMETER: &lt;PARAMETER NAME&gt;</p> <p>As explained in <a href="#">About the ENTER_PARAMETER Command on page 95</a>, specify a correct and complete Parameter Name, which should contain all the necessary parts of the general form:</p> <p>&lt;IDENTIFIER&gt;(&lt;PHASE&gt;,&lt;CONSTITUENT ARRAY&gt;;&lt;DIGIT&gt;)</p> <p>If a parameter name is not acceptable or &lt;Enter&gt;, is pressed, a message displays:</p> <p>*** Error, please re-enter each part separately</p> <p>and you are prompted for input for each required part for a parameter name.</p>
Options	Description or Information
IDENTIFIER	<p>IDENTIFIER (/X/): &lt;G OR L, OR TC, OR BM, OR V0 OR VA OR VB OR VC OR VK&gt;</p> <p>If this command is used one or more times, the previous value on this prompt is set as default. Press &lt;Enter&gt; for the same type identifier or specify a new type.</p>
PHASE NAME	<p>PHASE NAME (/ABCD/): &lt;PHASE NAME&gt;</p> <p>Each parameter is valid for a specific phase only. The name of that phase must be supplied (maximum 24 characters). The name can be abbreviated.</p>

Syntax	ENTER_PARAMETER
CONSTITUENT	<p>CONSTITUENT (IN SUBLATTICE # /ABC/) : &lt;SPECIES NAME&gt;</p> <p>A parameter is identified by the constituents on a specified sublattice site of the given phase, the stoichiometric coefficients of which are multiplied with the parameter. The name of the constituent can be abbreviated.</p> <p> It is the species name, not the stoichiometric formula required here.</p> <p>If this command is used one or more times, the previous value on this prompt is set as default. Accept it by pressing &lt;Enter&gt; if the constituent is the same, or specify a new species name.</p>
INTERACTING CONSTITUENT	<p>For phases with several sublattices, the program asks for one constituent in each sublattice.</p> <p>INTERACTING CONSTITUENT (IN SUBLATTICE # /XYZ/) : &lt;SPECIES NAME&gt;</p> <p>If this command is used one or more times, the previous value on this prompt is set as default. Press &lt;Enter&gt; to accept it if the constituent is the same, or specify a new species name.</p> <p> To cancel the default value of the interacting constituent type <b>NONE</b> or the name of another constituent.</p> <p>This question is repeated until all the interested interacting constituent(s) on a specific sublattice in the phase are specified, and finally an &lt;Enter&gt; is enforced.</p>
DEGREE	<p>DEGREE /#/: &lt;DEGREE&gt;</p> <p>Degree is model-dependent. Specify an integer number (a value from 0 through 9) as the degree of composition-dependent interaction contribution for the phase parameter. This is valid for excess energy (<math>L</math>), Curie temperature (<math>T_C</math>) and Bohr magneton number (<math>B_{MAGN}</math>), as well as for volume-related parameters (<math>V_0</math>, <math>V_A</math>, <math>V_B</math>, <math>V_C</math> or <math>V_K</math>).</p> <p>For binary interaction parameters, the degree is usually the power in the Redlich-Kister expression. For ternary interaction parameters, it is usually the Hillert ternary index.</p> <p>For a standard <math>G</math> parameter for a pure component (end-member) its degree should be always 0 and this prompt should not display.</p>
PHASE PARAMETER	<p>After this prompt, the program echoes on the screen the full TP-Function of the phase parameter.</p>



Syntax	ENTER_PARAMETER
	<p>LOW TEMPERATURE LIMIT /298.15/: &lt;LOWEST TEMPERATURE LIMIT IN K&gt;</p> <p>Specify the lowest temperature limit (in Kelvin), or the lowest-pressure limit (in Pascal but entered as a negative number), for the current TP-Function.</p> <p>FUNCTION: &lt;DEFINITION FOR A FUNCTION&gt;</p> <p>A TP-Function consists of terms in T and P.</p> <p>&amp; &lt;CONTINUATION OF THE DEFINITION FOR THE CURRENT FUNCTION&gt;</p> <p>Continuation of a TP-Function definition.</p> <p>HIGH TEMPERATURE LIMIT /6000/: &lt;HIGH TEMPERATURE LIMIT IN K&gt;</p> <p>Specify the high temperature limit (in Kelvin), or the high-pressure limit (in Pascal; only if the <i>lowest limit</i> is entered as a negative number) for the current TP-Function.</p> <p>ANY MORE RANGES /N/: &lt;Y OR N&gt;</p> <p>Enter Y for more function(s) or N to end this command.</p>

## LIST\_ALL\_VARIABLES

Create a list of the values and status of all variables in the PARROT workspace on screen or in a text file. After an optimization some statistical information is also written. The correlation matrix is written if that option is chosen.



Also see [SET\\_OUTPUT\\_LEVELS](#) on page 115.

Syntax	LIST_ALL_VARIABLES
Prompt	<p>OUTPUT TO SCREEN OR FILE /SCREEN/: &lt;FILE NAME&gt;</p> <p>A list of the current values and status, as well statistical information (if after optimization) and the correlation matrix (optionally), for all variables is written on screen (by pressing &lt;Enter&gt;) or on the list file under a specific file name which can later on be opened and edited by basic text editor.</p>
	<p><b>Example Output</b></p> <p>The following is the listed variables for the example TCEX36, after the first optimization when having set all variables available for optimization.</p> <pre> == OPTIMIZING VARIABLES ==  AVAILABLE VARIABLES ARE V1  TO V00  VAR.      VALUE              START VALUE      SCALING FACTOR    REL.STAND.DEV </pre>

Syntax	LIST_ALL_VARIABLES
	<pre> V1      2.03729090E+04      2.03688352E+04      2.03688352E+04 3.41524152E+00  V2      -2.94286372E+01      -2.94286372E+01      -2.94286372E+01 2.37944771E+00  V11     -2.17373936E+04      -2.18095983E+04      -2.18095983E+04      3.97086303E- 02  V12      1.52107184E+01      1.51660547E+01      1.51660547E+01      5.84552327E- 02  V15      2.42082351E+04      2.45139169E+04      2.45139169E+04 5.00914471E+00  V16      -8.38723972E+00      -8.83460472E+00      -8.83460472E+00 1.60961318E+01  V17      3.08916533E+03      3.15802558E+03      3.15802558E+03 9.63738108E+00  V19      2.20292586E+04      2.21385673E+04      2.21385673E+04 4.14274011E+01  V20     -7.04217974E+00      -7.22424882E+00      -7.22424882E+00 1.00561540E+02  NUMBER OF OPTIMIZING VARIABLES :      9  ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO  THE SUM OF SQUARES HAS CHANGED FROM      8.00002729E+04 TO      8.00002719E+04  DEGREES OF FREEDOM      45.  REDUCED SUM OF SQUARES      1.77778382E+03 </pre>

## LIST\_CONDITIONS

In the PARROT module, generate a list of the current values of optimization conditions, as well the current status of listing, either on screen or in a basic text file which can be opened and edited by a text editor.

Syntax	LIST_CONDITIONS
Prompt	<pre> OUTPUT TO SCREEN OR FILE /SCREEN/: &lt;FILE NAME&gt;  Press &lt;Enter&gt; to output to screen or on the list file under a specific file name. </pre>

## LIST\_PARAMETER


This command is for both the GIBBS and PARROT modules.

List the TP-function(s) of a specific parameter for a phase. You must supply the name of the phase parameter:

THE PARAMETER NAME: <IDENTIFIER> (<PHASE>, <CONSTITUENT ARRAY>; <DIGIT>)



For encrypted commercial databases, you may not be able to use this command to list any retrieved parameter.

Syntax	LIST_PARAMETER
Prompts	<p>PARAMETER: &lt;PARAMETER NAME&gt;</p> <p>Specify a correct and complete parameter name, which should contain all the necessary parts of the general form: &lt;identifier&gt;(&lt;phase&gt;,&lt;constituent array&gt;;&lt;digit&gt;)</p> <p> See <a href="#">About the ENTER_PARAMETER Command on page 95</a> to learn how to define the Parameter Name.</p> <p>If a parameter name is not acceptable or &lt;Enter&gt; is pressed, an error message displays:</p> <pre>*** Error, please re-enter each part separately</pre> <p>The program prompts for separate input for each required part for a parameter name.</p>
	<p>IDENTIFIER (/X/): &lt;G OR L, OR TC, OR BM, OR V0 OR VA OR VB OR VC OR VK&gt;</p> <p>Specify one of these types of legal identifiers.</p>
	<p>PHASE NAME (/ABCD/): &lt;PHASE NAME&gt;</p> <p>Specify the phase name.</p>
	<p>CONSTITUENT (IN SUBLATTICE # /ABC/): &lt;SPECIES NAME&gt;</p> <p>Specify the constituent name on the specified sublattice site of the given phase.</p>
	<p>INTERACTING CONSTITUENT (IN SUBLATTICE # /XYZ/): &lt;SPECIES NAME&gt;</p> <p>Specify the interacting constituent name on the specified sublattice site of the given phase; if there is no interacting constituent, press &lt;Enter&gt;.</p>
	<p>INTERACTING CONSTITUENT (IN SUBLATTICE # /XYZ/): &lt;SPECIES NAME&gt;</p> <p>If there is more than one interacting constituent on the specified sublattice site of the given phase, specify them; otherwise press &lt;Enter&gt;.</p>
	<p>DEGREE /#/: &lt;DEGREE&gt;</p> <p>Specify a numerical number as the degree for the phase parameter.</p>

## LIST\_PHASE\_DATA (from GIBBS)

All data for a specific phase are written on screen. The thermochemical parameters listed for each phase are always in SI units.

Syntax	LIST_PHASE_DATA
Prompt	<p>PHASE NAME: &lt;PHASE NAME&gt;</p> <p>Specify a phase name.</p>

## LIST\_RESULT

List the result of the current optimization run on screen or in a specified file. The level of detail listed can be prescribed by the command [SET\\_OUTPUT\\_LEVELS](#) on page 115.

The LIST\_RESULT command has an option **G** for creation of an experimental data file with two columns, one for the experimental value and the other for the calculated value. It allows plotting a diagram and visualizing the fitting results. The plot is automatically plotted and you can scale it giving commands in the POST module. The option **D** lists all experiments, including those with fulfilled inequalities which are suppressed with the default option **C**.

Syntax	LIST_RESULT
Prompt	<p>FULL, CONDENSED, DETAILED OR GRAPHIC FORMAT: /C/: &lt;C OR D OR F OR G&gt;</p> <p>Choose a format.</p> <ul style="list-style-type: none"> <li>• <b>C</b> (condensed) is the default.</li> <li>• <b>D</b> (detailed) lists all experiments, including those with fulfilled inequalities (not included with the default condensed file).</li> <li>• The <b>G</b> (graphical) format creates an experimental data file containing two columns, one with the experimental value and the other with the calculated value. This allows plotting of a diagram where all symbols should be on the diagonal if the fit is perfect. The plot is automatically plotted and you can scale it giving commands in the POST module.</li> <li>• The <b>F</b> (full) format is obsolete but retained for backward compatibility.</li> </ul> <p>OUTPUT TO SCREEN OR FILE /SCREEN/: &lt;FILE NAME&gt;</p> <p>A list of the current optimization results are written on screen (by pressing &lt;Enter&gt;) or on the list file under a specific file name which can later on be opened and edited by basic text editor.</p> <p>The output normally consists of these parts:</p> <ul style="list-style-type: none"> <li>• A title showing the data of the action;</li> <li>• A message on successful optimization with the iteration number in the last optimization;</li> </ul>

Syntax	LIST_RESULT
	<ul style="list-style-type: none"> <li>• A paragraph describing the optimization condition;</li> <li>• A list of the latest set of optimized and fixed variables;</li> <li>• A paragraph describing the optimization quality (some statistical information);</li> <li>• A correlation matrix for all optimizing variables (optionally shown, pre-set by the SET_OUTPUT_LEVELS command);</li> <li>• A list of all parameters (including their symbol names, status and current values or function expressions), and all phase descriptions (including phase name, model names, constituents, and phase's <math>G/L/TC/BM</math> expressions) pre-defined for each phase in the system (optionally shown, pre-set by the SET_OUTPUT_LEVELS command);</li> <li>• A paragraph describing the alternate equilibria (and possible error during optimization);</li> <li>• A detailed list on all the equilibrium points used in the current optimization. If the alternate-mode is used in the optimization, only an error value is shown. For normal-mode calculations, a list is shown for the experimental equilibrium numbers (first column) and corresponding original experimental data (second column, in the form <code>quantity = value</code>) which are used in optimization (i.e. non-zero weighted points). Such experimental data are by each point compared by the calculated value (third column) after the last optimization. Also listed are the experimental error (column 4), the difference between the calculated value and original experimental data (column 5), and the contribution to the sum of least square (column 6).</li> </ul>

### Example Output

The following is the listed result in the example TCEX36 ( in the *Console Mode Examples Guide.*), after the first optimization based on the prescribed definitions in the TCEX36a.TCM and TCEX36b.TCM, but having set all variables available for optimization.

```
=====
                        OUTPUT FROM P A R R O T.
=====
*** SUCCESSFUL OPTIMIZATION. ***          NUMBER OF ITERATIONS:  10
== OPTIMIZING CONDITIONS ==
RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
```

```

MINIMUM SAVE ON FILE: Y

ERROR FOR INEQUALITIES = 1.00000000E+00

RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04

ARGUMENTS FOR SUBROUTINE VA05AD (HSL)

  MAXFUN = 1  DMAX = 1.00000000E+02  H = 1.00000000E-04  ACC = (INITIAL SUM
OF SQUARES) * 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.    VALUE                START VALUE        SCALING FACTOR    REL.STAND.DEV
V1      2.03749463E+04        2.03729090E+04    2.03729090E+04    3.41455863E+00
V2      -2.94286372E+01       -2.94286372E+01   -2.94286372E+01   2.37944774E+00
V11     -2.17395673E+04       -2.17373936E+04   -2.17373936E+04   3.98405298E-02
V12     1.52107184E+01        1.52107184E+01    1.52107184E+01    5.82861832E-02
V15     2.42106560E+04        2.42082351E+04    2.42082351E+04    5.07239609E+00
V16     -8.38723972E+00       -8.38723972E+00   -8.38723972E+00   1.69546796E+01
V17     3.08947424E+03        3.08916533E+03    3.08916533E+03    9.85220694E+00
V19     2.20314615E+04        2.20292586E+04    2.20292586E+04    4.16329629E+01  V20    -
7.04217974E+00  -7.04217974E+00  -7.04217974E+00  1.03161466E+02

NUMBER OF OPTIMIZING VARIABLES : 9

ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO

THE SUM OF SQUARES HAS CHANGED FROM 8.00002719E+04 TO 8.00002709E+04

DEGREES OF FREEDOM 45. REDUCED SUM OF SQUARES 1.77778380E+03

Number of alternate equilibria 14

SYMBOL      STATUS  VALUE/FUNCTION
R           80000000  8.3145100E+00
RTLNP      20000000  +R*T*LN(1E-05*P)
V1          48000000  2.0374946E+04
V2          48000000  -2.9428637E+01
V11         48000000  -2.1739567E+04
V12         48000000  1.5210718E+01
V15         48000000  2.4210656E+04
V16         48000000  -8.3872397E+00
V17         48000000  3.0894742E+03
21 V19      48000000  2.2031462E+04  22 V20      48000000  -7.0421797E+00

LIQUID

EXCESS MODEL IS REDLICH-KISTER_MUGGIANU  CONSTITUENTS: A,B

G(LIQUID,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +14000-10*T

```

---

```

      G(LIQUID,B;0)-G(BCC,B;0) =      500.00<T< 2000.00: +18000-12*T
      L(LIQUID,A,B;0) =      500.00<T< 2000.00: +V11+V12*T      L(LIQUID,A,B;1) =
500.00<T< 2000.00: +V13+V14*T
A2B
      2 SUBLATTICES, SITES 2: 1      CONSTITUENTS: A : B
      G(A2B,A;B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =
      500.00<T< 2000.00: +V1+V2*T+V3*T*LN(T)
BCC
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU      CONSTITUENTS: A,B
      G(BCC,A;0)-G(BCC,A;0) =      500.00<T< 2000.00: 0.0
      G(BCC,B;0)-G(BCC,B;0) =      500.00<T< 2000.00: 0.0
      L(BCC,A,B;0) =      500.00<T< 2000.00: +V15+V16*T
      L(BCC,A,B;1) =      500.00<T< 2000.00: +V17+V18*T
FCC
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU      CONSTITUENTS: A,B
      G(FCC,A;0)-G(BCC,A;0) =      500.00<T< 2000.00: 408
      G(FCC,B;0)-G(BCC,B;0) =      500.00<T< 2000.00: +3300-3*T
      L(FCC,A,B;0) =      500.00<T< 2000.00: +V19+V20*T
      L(FCC,A,B;1) =      500.00<T< 2000.00: +V21+V22*T
=====  BLOCK NUMBER 1
DEFINED CONSTANTS
      DX=2E-2, P0=101325, DH=500, DT=10
DEFINED FUNCTIONS AND VARIABLES%
      HTR=HM(LIQUID)-HM(A2B)
Alternate equilibrium calculation      0.4183
Alternate equilibrium calculation      0.1932
Alternate equilibrium calculation      0.1016
Alternate equilibrium calculation      1.4354E-03
Alternate equilibrium calculation      2.5063E-02
Alternate equilibrium calculation      8.3929E-03
Alternate equilibrium calculation      141.4
Alternate equilibrium calculation      141.4
Alternate equilibrium calculation      141.4
Alternate equilibrium calculation      141.4
Alternate equilibrium calculation      1.2532E-03
Alternate equilibrium calculation      5.4781E-04

```

---

```

Alternate equilibrium calculation          1.5404E-03
Alternate equilibrium calculation          1.2702E-03
ACR (B)=9.4E-1          0.9397          2.85E-02 -2.7745E-04 -9.7472E-03
ACR (B)=8.4E-1          0.8395          2.82E-02 -4.9038E-04 -1.7396E-02
ACR (B)=7.4E-1          0.7407          2.81E-02  7.3804E-04  2.6305E-02
ACR (B)=6.4E-1          0.6424          2.81E-02  2.3935E-03  8.5272E-02
ACR (B)=5.4E-1          0.5434          2.82E-02  3.4449E-03  0.1220
ACR (B)=4.4E-1          0.4428          2.85E-02  2.8265E-03  9.9024E-02
ACR (B)=3.4E-1          0.3394          2.90E-02 -5.8174E-04 -2.0040E-02
ACR (B)=2.3E-1          0.2320          2.97E-02  2.0260E-03  6.8208E-02
ACR (B)=1.2E-1          0.1194          3.06E-02 -6.4192E-04 -2.0981E-02
HMR (LIQUID)=-1964      -1957.          5.00E+02   7.439          1.4878E-02
HMR (LIQUID)=-3500      -3478.          5.00E+02  21.67          4.3338E-02
HMR (LIQUID)=-4588      -4565.          5.00E+02  22.69          4.5382E-02
HMR (LIQUID)=-5239      -5217.          5.00E+02  21.50          4.3008E-02
HMR (LIQUID)=-5454      -5435.          5.00E+02  19.11          3.8216E-02
HMR (LIQUID)=-5233      -5217.          5.00E+02  15.50          3.1008E-02
HMR (LIQUID)=-4575      -4565.          5.00E+02   9.691          1.9382E-02
HMR (LIQUID)=-3481      -3478.          5.00E+02   2.669          5.3385E-03    118 HMR
(LIQUID)=-1950          -1957.          5.00E+02  -6.561         -1.3122E-02

```

## LIST\_STORE\_FILE

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

## LIST\_SYMBOL\_IN\_GES

Lists TP-function(s) for the entered model parameters for phases in the system on screen. In many cases, the optimizing variables are parts of the TP-functions which in turn are entered in model parameters for various phases in the GIBBS workspace.

This command is a way to find out how the functions depend on the optimizing variables. In the PARROT module the list is only shown on screen, not written to any file (which the LIST\_SYMBOL command in the GIBBS module does).



Syntax	LIST_SYMBOL_IN_GES
Prompt	NAME: <SYMBOL NAME>  Specify a symbol name.  <input checked="" type="checkbox"/> Only those symbols that match this name are listed. Or press <Enter> for a list of all available symbols entered in the system.

## OPTIMIZE\_VARIABLES


Perform variable optimization. All system-definition data needed for the optimization is read from the current work file (\*.PAR). The result of the optimization is automatically stored in the current work file.

Syntax	OPTIMIZE_VARIABLES
Prompt	NUMBER OF ITERATION /N/: <INTEGRAL NUMBER OF ITERATION>  Specify an integral number for the optimization iteration. The specified iteration number is shown as the default number. The PARROT module tries this number of different sets of values of the optimizing variables unless it has converged earlier, or has given up earlier.
	<input checked="" type="checkbox"/> It initially takes a small step in each variable to find the steepest slope. You can give zero iteration to calculate the error in all selected experiments, and then use <a href="#">LIST_RESULT on page 104</a> to check how good (bad) the current fit is.

## READ\_PARROT\_WORKSPACES

Read the previous PARROT/GIBBS/POLY3 workspaces back to replace the current PARROT/GIBBS/POLY3 workspaces. It is useful if late changes made through various PARROT/GIBBS/POLY commands are not satisfactory.


Syntax	READ_PARROT_WORKSPACES
	The previous PARROT/GIBBS/POLY3 workspaces are always associated with the latest action to either open a work file by <a href="#">SET_STORE_FILE on page 116</a> , or to create a work file by <a href="#">CREATE_NEW_STORE_FILE on page 94</a> (either interactively in the PARROT module or through a <a href="#">MACRO_FILE_OPEN on page 5</a> of an *SETUP.TCM file), or to update the work file by <a href="#">SAVE_PARROT_WORKSPACES on page 111</a> .
	Unlike the READ commands in other modules (e.g. GIBBS or PLOY), this command in the PARROT module does not ask for the file name where to read a previously opened/created/updated PARROT/GIBBS/POLY3 workspaces, for the reason described above.

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

## RECOVER\_VARIABLES

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

## REINITIATE



	This command should not be used unless you want to destroy the current PARROT workspace. However, this PARROT command does not reinitiate the GIBBS/POLY3 workspaces.
---	---

Syntax	REINITIATE
	The workspace used by the PARROT program is reinitiated. All output and optimizing conditions are given their default values. All variables are set fixed with their value equal to zero.

## RESCALE\_VARIABLES

Syntax	RESCALE_VARIABLES
	The current values of all the parameters are copied to their start values and the scaling factors for further optimization. Thus it should be done now and again, in particular if you think the optimization results are improved after the previous run(s), or if any variable changes more than a factor of 10.

## SAVE\_PARROT\_WORKSPACES

Syntax	SAVE_PARROT_WORKSPACE
	<p>If the latest changes made through various PARROT/GIBBS/POLY commands are as required, use this command to save the current workspace (i.e. data area) used by the PARROT program (also including the current GIBBS and POLY3 workspaces), onto the present work *.PAR file which has already been opened by <a href="#">SET_STORE_FILE</a> on page 116 or been created by <a href="#">CREATE_NEW_STORE_FILE</a> on page 94 (either interactively in the PARROT module or through a MACRO_FILE_OPEN of an *SETUP.TCM file).</p> <p> The PARROT/GIBBS/POLY3 workspaces are updated after each PARROT/GIBBS/POLY command. This means the current PARROT/GIBBS/POLY3 workspaces are always updated onto the latest work *.PAR file that is associated with the latest SET_STORE_FILE or CREATE_NEW_STORE_FILE command.</p> <p> Unlike the SAVE commands in other modules (e.g. GIBBS or PLOY), this command in the PARROT module does not ask for the file name where to save the current PARROT/GIBBS/POLY3 workspaces, for the reason described above. You cannot use this command if there is no work *.PAR file opened or created already.</p>

## SET\_ALTERNATE\_MODE

Turn the alternate mode on or off. The alternate mode is described in [PARROT Commands](#) on page 86. It should be used only to optimize start values of the model parameters in the beginning of the assessment.

With the ALTERNATE mode is possible to include functions to be evaluated together with an alternate calculation and to select ALTERNATE mode for each experimental equilibrium.

Syntax	SET_ALTERNATE_MODE
Prompt	<p>ON /Y/: &lt;Y OR N&gt;</p> <p>The default Y turns on the alternate mode.</p>

## SET\_EXTERNAL\_PARAMETER

Optimize model parameters of the so-called external models, which may not be as fully-implemented/integrated parts inside the GIBBS system and thus are independently defined within user-specified/written source codes. This command makes links between the PARROT optimizing variables and external model parameters.



In order to be able to build the specified external model and to use this SET\_EXTERNAL\_PARAMETER command, it requires you to first write codes for a preferred external model (as it is not within the standard GIBBS system of the Thermo-Calc software) and then provide it to the consultancy team ([consult@thermocalc.se](mailto:consult@thermocalc.se)) of Thermo-Calc Software Company in Stockholm for the purpose of including the external model in a separate DLL that is interactively connected to the Thermo-Calc software. Such a special service can/should only be provided under the restrictive condition that a specific Consultancy Project Contract is bilaterally agreed and signed in advance between users and Thermo-Calc Software.

Syntax	SET_EXTERNAL_PARAMETER
Prompt	EXTERNAL NAME: <PARAMETER NAME IN THE EXTERNAL MODEL> Correctly specify the parameter name defined within a specified/written external model.
	AS OPTIMIZING VARIABLE NUMBER: <N> Give the number of the PARROT optimizing variable, which should have a unique link to the specified parameter name of the external model. For example, @@ Link PARROT variables to CAM parameters: SET-EXTER-PAR GT (SLAG_A, O-2, SI+4, CA+2) 1 SET-EXTER-PAR ET (SLAG_A, O-2, SI+4, CA+2) 2 SET-EXTER-PAR EXT (SLAG_A, O-2, SI+4, CA+2) 3

## SET\_FIX\_VARIABLE

Prescribe a fixed value to a variable. The variable is considered as a constant at the optimization, usually after successful optimization runs for some specific variables (for some of the phases in the system). Such fixed variables can also be set back for further optimization run by using [SET\\_OPTIMIZING\\_VARIABLE](#) on page 114.

Syntax	SET_FIX_VARIABLE
Prompts	VARIABLE NUMBER: <VARIABLE NUMBER(S)> Specify the number of the variable. It is possible to give a range by giving two numbers with a hyphen in between (no spaces allowed), e.g. 1. The parameters within the limits are set fixed to their current values (no question of values).
	START VALUE /XXXX.XXXXX/: <A VALUE TO BE FIXED> Specify a numerical value to be fixed for the selected variable (only when one variable number is specified at the previous prompt). The current value for the selected variable is

Syntax	SET_FIX_VARIABLE
	<p>shown as default.</p> <p>If a range of variable numbers is specified at the previous prompt, this question is not prompted, and the current values are used as fixed values.</p>

## SET\_OPTIMIZING\_CONDITION

Specify the conditions for the optimization. The default values are chosen automatically by the PARROT program, and in most cases these should not be changed.



The optimization stops when the sum of errors decreases by this value, even though it might be possible to increase it further with a new OPTIMIZE command.


Syntax	SET_OPTIMIZING_CONDITION
	<p>RELATIVE STANDARD DEVIATION FOR EXPERIMENTS? /N/: &lt;Y OR N&gt;</p> <p>Choose whether the standard deviation of the experimental determinations are absolute values (N) or if these are used as relative weighting factors (Y). The estimated standard deviations of the optimized variables might be different for the two cases.</p>
Prompt	<p>MIN SAVE ON FILE? /Y/: &lt;Y OR N&gt;</p> <p>Specify whether the program should minimize the transfer of data to and from the current work file during the optimization:</p> <p>If Y, it speeds up the optimization. After optimization use the <a href="#">SAVE_PARROT_WORKSPACES on page 111</a> command to update the progress onto the current work file.</p> <p>If minimum saving on file is not specified (N), the workspaces are stored on the current work file after every iteration in the optimization procedure.</p>
	<p>ERROR FOR VARIABLE BOUNDS: /1/: &lt;RETURN &gt;</p> <p>This feature has not been implemented yet. Press &lt;Enter&gt;.</p>
	<p>RELATIVE STEP FOR CALCULATION OF DERIVATIVES: /1E-04/: &lt;XXX&gt;</p> <p>In the calculation of the correlation matrix for equilibria with inaccuracy in the independent state variables, some numerical derivatives might have to be calculated.</p> <p>Specify the relative step (xxx) for the calculation of these derivatives.</p>
	<p>MAXFUN (VA05AD): /100/: &lt;N&gt;</p> <p>The maximum number of iterations in the optimization. The same value set by the OPTIMIZE command.</p>

Syntax	SET_OPTIMIZING_CONDITION
	<p>DMAX (VA05AD) : /100/: &lt;N&gt;</p> <p>An estimate of the maximum distance between the start and the final values of the variables. A smaller value makes the program vary the parameters with smaller factors.</p>
	<p>H (VA05AD) : /1E-04/: &lt;XXX&gt;</p> <p>The step used in the scaled variables for calculating numerical derivatives during the optimization.</p>
	<p>ACC/(INITIAL SUM OF SQUARES) (VA05AD) : /.001/: &lt;XXX&gt;</p> <p>The break condition for the optimization. The accepted value is the difference between the true minimum and the calculated one.</p>

## SET\_OPTIMIZING\_VARIABLE

Specify which variable value should be estimated at the optimization. Such a variable can have a value of zero or another start value, or is fixed by [SET\\_FIX\\_VARIABLE](#) on page 112 prior to the previous optimization run.

For a good reference prior to this command, a list of all variables (which are used to define various parameters for phases in the optimizing system, as pre-entered in the \*SETUP.TCM file or interactively entered in the GIBBS module) are obtained by using [LIST\\_ALL\\_VARIABLES](#) on page 101.

Syntax	SET_OPTIMIZING_VARIABLE
Prompts	<p>VARIABLE NUMBER: &lt;VARIABLE NUMBER(S)&gt;</p> <p>Specify the number(s) for the variable(s) to be set. Any non-zero parameter within the range is allowed to be optimized. A parameter with a current value equal to zero must be specified explicitly here in order to be optimized.</p> <p>Specify a range by giving two numbers connected by a hyphen (no space allowed!), e.g. 2-8. Under this circumstance, no question of start values are asked.</p>
	<p>START VALUE /XXXX.XXXXX/: &lt;A GUESS VALUE&gt;</p> <p>Specify a start guess of the optimum value (only when one variable number is specified at the previous prompt). The current numerical value for the selected variable is shown as default.</p> <div style="border: 1px solid black; padding: 10px; margin-top: 10px;">  <p>This guess is critical as the initial guess of all parameters must make it possible to calculate the selected equilibria. If a range of variable numbers is specified at the previous prompt, this question is not prompted, and the current values (as start values) are not changed.</p> </div>

## SET\_OUTPUT\_LEVELS


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

Syntax	SET_OUTPUT_LEVELS
Prompts	<p>LIST INCREMENT /1/: &lt;INCREMENT IN ITERATION NUMBER&gt;</p> <p>Specify the increment in iteration number for which information is listed on screen during the optimization. By giving a larger number it shortens the list.</p>
	<p>LIST SUM OF SQUARES: /Y/: &lt;Y OR N&gt;</p> <p>Choose whether the sum of squares is listed on screen during the optimization procedure.</p>
	<p>LIST SCALED VARIABLES: /Y/: &lt;Y OR N&gt;</p> <p>Choose whether the scaled variable values are listed on the terminal during the optimization procedure.</p>
	<p>LIST WEIGHTENED RESIDUALS: /N/: &lt;N OR Y&gt;</p> <p>Choose whether the weighted residuals are listed on the terminal during the optimization procedure.</p>
	<p>LIST ALL PARAMETERS: /N/: &lt;N OR Y&gt;</p> <p>Choose whether all parameters in the models are listed in <a href="#">LIST_RESULT</a> on page 104.</p>
	<p>LIST CORRELATION MATRIX: /N/: &lt;N OR Y&gt;</p> <p>Choose whether the correlation matrix of the variables are listed with the commands LIST_RESULT and <a href="#">LIST_ALL_VARIABLES</a> on page 101.</p>

## SET\_SCALED\_VARIABLE

This command is similar to [SET\\_OPTIMIZING\\_VARIABLE](#) on the previous page in that it specifies start values for optimizing variables. The difference being it is functional for only one optimizing variable at one time. It also prescribes a minimum and maximum value for the variable. During the optimization runs, the variable value is limited within this min-max range.

Such a variable may have a value of zero or another start value, or may be fixed by [SET\\_FIX\\_VARIABLE](#) on page 112 prior to the previous optimization run. For a good reference prior to using this command, a list of all variables (which are used to define various parameters for phases in the optimizing system, as entered in the \*SETUP.TCM file or interactively entered in the GIBBS module) is obtained by using [LIST\\_ALL\\_VARIABLES](#) on page 101.

Syntax	SET_SCALED_VARIABLE
Prompts	<p>VARIABLE NUMBER: &lt;VARIABLE NUMBER(S)&gt;</p> <p>Specify the number for an optimizing variable to be set. Any non-zero parameter is allowed to be optimized, and a parameter with a current value equal to zero must be specified explicitly here in order to be optimized.</p>
	<p>START VALUE /XXXX.XXXXX/: &lt;A GUESS VALUE&gt;</p> <p>Specify a start guess of the optimum value. The current numerical value for the selected variable is shown as default.</p> <div style="border: 1px solid black; background-color: #d4edda; padding: 10px; margin-top: 10px;">  <p>This guess is critical as the initial guess of all parameters must make it possible to calculate the selected equilibria.</p> </div>
	<p>MIN VALUE /XXXX.XXXXX/: &lt;A GUESS VALUE&gt;</p> <p>Specify a minimum guess of the optimum value. It should be smaller than, at least equal to, the current start value for the selected variable.</p>
	<p>MAX VALUE /XXXX.XXXXX/: &lt;A GUESS VALUE&gt;</p> <p>Specify a maximum guess of the optimum value. It should be larger than, at least equal to, the current start value for the selected variable.</p>

## SET\_STORE\_FILE

Specify a store file (work file) to be used for compilation and optimization. The \*.PAR work file must be created ([CREATE\\_NEW\\_STORE\\_FILE on page 94](#)) as a store file. The GIBBS, POLY and PARROT workspaces are read from the specified store file (with a default extension of PAR).

Syntax	SET_STORE_FILE
Prompt	<p>Enter an *.PAR file name in the <b>File name</b> field and specify the working directory in the <b>Look in</b> field. Normally the default file-type in the <b>Files of type</b> field is the correct one for the PARROT workspace format (i.e. *.PAR file). Click <b>Open</b> or <b>Cancel</b> as applicable.</p>



## POLY\_3 Commands

In this section:

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<i>ADD_INITIAL_EQUILIBRIUM</i> .....	119
<i>ADVANCED_OPTIONS</i> <i>Descriptions</i> .....	120
<i>ADVANCED_OPTIONS</i> .....	125
<i>AMEND_STORED_EQUILIBRIA</i> .....	133
<i>CHANGE_STATUS</i> .....	135
<i>COMPUTE_EQUILIBRIUM</i> .....	139
<i>COMPUTE_TRANSITION</i> .....	141
<i>CREATE_NEW_EQUILIBRIUM</i> .....	143
<i>DEFINE_COMPONENTS</i> .....	143
<i>DEFINE_DIAGRAM</i> .....	144
<i>DEFINE_MATERIAL</i> .....	147
<i>DELETE_INITIAL_EQUILIBRIUM</i> .....	151
<i>DELETE_SYMBOL</i> .....	151
<i>ENTER_SYMBOL</i> .....	151
<i>EVALUATE_FUNCTIONS</i> .....	155
<i>LIST_AXIS_VARIABLE</i> .....	155
<i>LIST_CONDITIONS</i> .....	155
<i>LIST_EQUILIBRIUM</i> .....	156
<i>LIST_INITIAL_EQUILIBRIA</i> .....	157
<i>LIST_STATUS</i> .....	157
<i>LIST_SYMBOLS</i> .....	158
<i>LOAD_INITIAL_EQUILIBRIUM</i> .....	158
<i>MAP</i> .....	158
<i>POST</i> .....	160
<i>READ_WORKSPACES</i> .....	160

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<i>RECOVER_START_VALUES</i> .....	<i>160</i>
<i>REINITIATE_MODULE</i> .....	<i>161</i>
<i>SAVE_WORKSPACES</i> .....	<i>161</i>
<i>SELECT_EQUILIBRIUM</i> .....	<i>162</i>
<i>SET_ALL_START_VALUES</i> .....	<i>162</i>
<i>SET_AXIS_VARIABLE</i> .....	<i>164</i>
<i>SET_CONDITION</i> .....	<i>165</i>
<i>SET_INPUT_AMOUNTS</i> .....	<i>168</i>
<i>SET_NUMERICAL_LIMITS</i> .....	<i>168</i>
<i>SET_REFERENCE_STATE</i> .....	<i>169</i>
<i>SET_START_CONSTITUTION</i> .....	<i>171</i>
<i>SET_START_VALUE</i> .....	<i>171</i>
<i>SHOW_VALUE</i> .....	<i>172</i>
<i>STEP_WITH_OPTIONS</i> .....	<i>172</i>
<i>TABULATE</i> .....	<i>187</i>

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## ADD\_INITIAL\_EQUILBRIUM

Add initial equilibrium points from which a phase diagram is calculated (through the [MAP](#) on page 158 command).

Syntax	ADD_INITIAL_EQUILBRIUM
	<p><code>DIRECTION /DEFAULT/: &lt;DIRECTION CODE&gt;</code></p> <p>direction code (s) 1 or 2 for positive direction of axis 1 or 2, respectively; -1 or -2 for negative direction of axis 1 or 2, respectively; Default for all directions.</p>
Prompt	<p>The direction is important when the initial equilibrium point is in a single-phase region or when the phase diagram is an isopleth (tie-lines not in the plane of calculation). In such cases, the program searches for a line in the diagram (i.e. a line where the amount of a phase is zero, imply that if it starts to become stable on one side of the line and disappear on the other side) in the given direction.</p>

Normally, this command is not needed to calculate a property diagram (with the [STEP\\_WITH\\_OPTIONS](#) on page 172 → `NORMAL` command-sequence). In many cases, the `ADD_INITIAL_EQUILBRIUM` command is not required for `MAP` commands either, as the mapping procedure starts from the current equilibrium state already calculated. In order to calculate a simple phase diagram, set the equilibrium conditions and the mapping axis variables, and then give a `MAP` command. But if a phase diagram has disconnected lines, the `ADD_INITIAL_EQUILBRIUM` command may still be needed to add two or more initial equilibria so that the `MAP` calculation starts from such initial equilibria at the specified directions to find all phase boundary lines.

This command becomes unnecessary in most cases, as the `MAP` routines that by default use the Global Minimization Technique handles all the initial equilibrium points in a robust and automatic way. Therefore, you do not need to have a good guess of the starting point and to add any initial equilibrium point prior to the calculations of various types of phase diagrams. However, if preferred, use this command to add any initial equilibrium points in certain directions, the `POLY` module uses the specified starting point(s) and corresponding user-added initial equilibrium point(s) for a mapping calculation; in such a case, the automatic procedure in the rewritten `MAP` routines are not enforced while the Global Minimization Technique can still be applied. Similar situations occur when a specific database, in which there are some definitions of initial-equilibrium adding direction(s) for accessed binary and/or ternary subsystems in its `ACCESSED_SYSTEM` section, is used in the `BINARY` or `TERNARY` module for calculating a binary or ternary phase diagram.

The `ADD_INITIAL_EQUILBRIUM` command with the default direction scans along the axis variables and generates start points each time the scanning procedure crosses a phase boundary. In addition, it generates four start points, scanning cross the middle of each axis, if there is any solubility line that does not reach the axes. At the `MAP` command, a search for lines in the diagram is made along each direction of the axis variables in the diagram. In this way, it should guarantee that all possible phase boundary lines in a phase diagram are found. Of course, it may take a little longer time to execute than using the minimum number of start points, as some lines may be calculated more than once. But the `POLY` module

remembers all node points and subsequently stops calculations along a line when it finds a known node point.

It is also possible to create a sequence of start points from one initial equilibria by appending a > after the direction at the ADD command. For example:

```
Direction /default/: 2>
Direction /default/: -2>
```

This generates one start point for each set of phase change in the positive direction of the axis 2 (or negative direction of the axis 2); this ensures finding all possible phase boundary lines (not just the first one) along such an axis direction.

This is particularly useful when you have a phase diagram with several lines with no intersection. It is thus possible to calculate e.g. an isopleth for a much more limited composition range. It is also useful for calculating CVD diagrams and Pourbaix diagrams.

All the initial equilibrium points generated by the ADD\_INITIAL\_EQUILIBRIUM command (previously and presently; saved in the current POLY workspace) can be easily listed out on screen with [LIST\\_INITIAL\\_EQUILIBRIA on page 157](#). A certain initial equilibrium point (including its conditions and equilibrium results) can be loaded into the current equilibrium, if needed, with [LOAD\\_INITIAL\\_EQUILIBRIUM on page 158](#). Any specific or all of the initial equilibrium points can be deleted from current POLY workspace, if desired, with [DELETE\\_INITIAL\\_EQUILIBRIUM on page 151](#).

## ADVANCED\_OPTIONS Descriptions



Also see [ADVANCED\\_OPTIONS on page 125](#) for information about the command.

These ADVANCED\_OPTIONS can be set:

### EQUILIBRIUM\_CALCUL

Designed to decide how to perform the Ordinary POLY Minimization (i.e. the traditional Gibbs Energy Minimization) in the POLY module. By default, the Global Minimization Technique for various single point equilibrium calculations and for stepping or mapping calculations is used. You can use the advanced option [GLOBAL\\_MINIMIZATION on page 236](#) to permanently turn off (for all sequential calculations throughout the current TCC run) the Global Minimization Technique and consequently use only the Ordinary POLY Minimization, and additionally adjust the ways to proceed the normal minimization (mainly in terms of how to control the steps in reaching Gibbs energy minima in an equilibrium state). When enforcing the Global Minimization Technique in the equilibrium calculations, you can further adjust the manners for assigning grid-points and for handling new possible compositional set(s) for solution phases during stepping/mapping; since the Global Minimization Technique also uses the normal POLY optimization routine for some calculations, it is also possible to change the ways on how to control the steps in reach Gibbs energy minima in an equilibrium state, in order to improve convergence.

### GLOBAL\_MINIMIZATION

Designed to decide how to perform the so-called Global Minimization in the POLY module. By default,

the POLY module uses the Global Minimization Technique for various single-point equilibrium calculations and for stepping or mapping calculations. You can use this to permanently (for all sequential calculations throughout the current TCC run) turn off the Global Minimization Technique and consequently use only the Ordinary POLY Minimization, and additionally adjust the ways to proceed the normal minimization (mainly in terms of how to control the steps in reaching Gibbs energy minima in an equilibrium state). When enforcing the Global Minimization Technique in the equilibrium calculations, you can adjust the manners for assigning grid-points and for handling new possible compositional set(s) for solution phases during stepping/mapping; since the Global Minimization Technique also uses the normal POLY optimization routine for some calculations, it is also possible to change the ways on how to control the steps in reach Gibbs energy minima in an equilibrium state, in order to improve convergence.

---

## LIST\_PHASE\_ADDITION

The values set as additional contributions (given by PHASE\_ADDITION) to Gibbs energy  $G_m$  (J/mol formula unit) to all the phases (stoichiometric or solution) are listed at the current calculated equilibrium.

## MAJOR\_CONSTITUENTS

Use this to set the major constituent(s) of a composition sets in a miscibility gap of a solution phase. Normally, the major constituents are specified when a new composition set is created by the NEW\_COMPOSITION\_SET option; but for the first composition set, this option may be needed before using NEW\_COMPOSITION\_SET.

## NEW\_COMPOSITION\_SET

A solution phase that can exist with two (or more) different compositions simultaneously must have two (or more) composition sets in its phase descriptions. Normally the database creates as many composition sets as is necessary but use this command to add or delete more composition sets. A complex solution phase in a defined multicomponent system can have up to 9 different composition sets for the purpose of appropriately handling its possible miscibility gap(s) under various temperature-pressure-composition conditions.

This option is unnecessary if the Global Minimization Technique is in use, as it can automatically detect all possible miscibility gap(s) for complex solution phases (normal or disordered/ordered phases) and then automatically add required composition sets for such phases in the defined system.

This option can automatically create composition sets also for disordered phase when it is executed for the ordered phase.

If you have your own data file, this option must be used to indicate that a solution phase can have a miscibility gap (or may exhibit some complex phase separations as to more than two composition sets), unless that the possibly-additional composition set(s) for the solution phase must have already been added inside the TDB file (through a TYPE\_DEFINITION command to amend composition-set) or been manipulated through the GIBBS module (using the AMEND\_PHASE\_DESCRIPTION COMPOSITION\_SET command-sequence). This option asks for default major constituents for the new sets and it is important that this is set correctly, otherwise the test for miscibility gaps may fail.

## OUTPUT\_FILE\_FOR\_SHOW

The name of a text file is asked for and all the results output from the command SHOW\_VALUE is written to this file.

## PARAEQUILIBRIUM

This calculates a paraequilibrium between two specific phases in an alloy system with one or more interstitial component(s) as fast diffusion species. Under the paraequilibrium state, two partially-equilibrated phases have the same chemical potential (but different contents) for one or more interstitial components (such as C, N, O, S, etc., as individual or combined)], along varied temperature or along a composition variable (of the matrix or one substitutional component) which has already set as the stepping variable with [SET\\_AXIS\\_VARIABLE](#) on [page 164](#).

To ensure a successful point calculation of paraequilibrium state between two specific phases in a defined alloy system, it is important that you first have made a single-point equilibrium calculation with an initial overall composition in the current system before performing this advanced-option calculation; however, it is unnecessary to obtain an equilibrium in which either one or both of the target phases is stable. The initial overall composition must have a reasonable setting for the desired paraequilibrium calculation for the two target phases. This is especially true for cases where there are more than one interstitial components to be considered in the paraequilibrium state, because different interstitial components (for example C and N combined) may have significant different behaviours as partitioning into different structured phases; otherwise, for one chosen interstitial component the initial overall composition is OK for the paraequilibrium calculation between the specified two phases, but for other chosen interstitial component(s) it might be impossible to calculate the paraequilibrium state.

Note the following:

Always check if the chosen phases A and B have the exactly same definition of elements and if the chosen interstitial components are all in the vacancy sublattice sites of the two phases; otherwise the program cannot find the paraequilibrium state (as it is impossible to correctly calculate u-fractions).

Always have a comprehensive understanding of the normal phase diagram for the currently investigated system, so that you make the appropriate choice of the phase pair and starting bulk composition for the system.

Always set the status of the chosen interstitial components as SPECIAL using the POLY command:

[CHANGE\\_STATUS on page 135](#) `Component <interstitial component> = SPECIAL`. By doing this, you get a clear picture of u-fractions of various substitutional and interstitial components, which are different from the overall composition in the system. The SPECIAL status means that specified component(s) are not included in summations for mole or mass fractions. Therefore, all the composition variables plotted from paraequilibrium calculations are u-fraction related quantities.

## PHASE\_ADDITION

Sometimes it is interesting to add a constant contribution to the Gibbs energy of a phase (stoichiometric or solution). This can be done in the Database Module (DATA) or Gibbs Energy Module (GIBBS), for a stoichiometric phase, or for a pure end-member in a solution phase. However, if the addition is related to the equilibrium state, for example, strain energies or surface energies, interfacial energies or deformation energies, it may be more convenient to have this quantity related to the equilibrium state rather than the thermodynamic data.

Give a value of an addition to the Gibbs energy of a phase. The value should always be constant (implying that the addition is not a function of phase composition or temperature-pressure conditions in the equilibrium state) and always be given in the unit of J/mol formula unit of the phase.

## PRESENT\_PHASE

The phase specified must be stable at all equilibria calculated during a [MAP on page 158](#) command. It is a way to limit the calculations of the monovariant lines in a ternary system to those in the liquidus surface. Normally such a calculation would have two compositional axes and a temperature axis and all monovariant lines, also those between 3 solids, would be mapped. If the liquid is set as PRESENT, only

those with the liquid is mapped.

### SHOW\_FOR\_T=

Display various thermodynamic properties (state variables, derived/partial variables or entered symbols) of the currently calculated (stable/meta-stable) equilibrium state but under a different temperature condition. This is useful for knowing, for example, a volume-related property of a frozen (stable/meta-stable) equilibrium state at a certain temperature, where the equilibrated phase assemblage and all the phase compositions are not adjusted while only the temperature condition is changed.

Use this option carefully. You must have successfully calculated a real equilibrium state under one temperature condition (normally the temperature for the last heat treatment). This can then be used to obtain the value(s) of any specified state variable(s) or derived/partial variable(s) or defined symbol(s) for thermodynamic properties of the entire system, of components, or of phases for the currently-defined system (being in a frozen state) under another temperature (normally at room temperature). No real equilibrium is re-calculated through this option, and thus the phase amounts and compositions in the system are the same as at the last real equilibrium calculation.

### STABILITY\_CHECK

In some composition ranges of a multicomponent system, it often happens that an unstable solution phase region locates inside a miscibility gap, and the stability limit (the *spinodal curve* or *spinodal*) may be not easy to find. A system inside a spinodal is thermodynamically unstable with respect to compositional fluctuations, and the system may experience the *spinodal decomposition* (i.e. decomposing to a mixture of regions with the two stable compositions, one on each side of the miscibility gap).

This option makes it possible to automatically check internal stability of both stable and unstable phases in all subsequent single-point equilibrium and MAP/STEP calculations. It can find out if any phase is subject to spinodal decomposition during the subsequent calculations. If there is an unstable phase located inside a miscibility gap in a calculation, it gives a warning so that you suspend the unstable phase, or use FORCED automatic start values for phase constituents (i.e. [SET\\_ALL\\_START\\_VALUES](#) on [page 162](#) → `FORCE` command-sequence), or create other composition sets; you can also ignore the warning message if you know that the unstable phase is not formed in the current calculations.

### STEP\_AND\_MAP

This is the default and is used to determine how to perform Global Minimization test and how to handle initial equilibrium points.

### T-ZERO\_TEMPERATURE

This calculates the temperature when two specific phases have the same Gibbs energy, i.e. the so-called T0 temperature. You must calculate an equilibrium state at an estimated temperature before performing this advanced-option calculation; however, it is unnecessary to obtain an equilibrium state in which either one or both of the target phases is stable.

### TOGGLE\_ALTERNATE\_MODE

Toggle the ALTERNATE mode for experimental equilibrium calculation between DEFAULT, ALWAYS and



NEVER, during data-assessments using the PARROT optimization.

## ADVANCED\_OPTIONS



Also see [ADVANCED\\_OPTIONS Descriptions on page 120](#).


Syntax	ADVANCED_OPTIONS
Prompt	WHICH OPTION? /STEP_AND_MAP/: <OPTION>
Options	Description and Information
NONE	<p>Take away any set advanced option in all subsequent single-point equilibrium and MAP/STEP calculations.</p> <p>If there is any convergence problem in finding a stable solution, at any stage of an advanced option calculation conducted by an ADVANCED_OPTIONS command-sequence, these messages display:</p> <pre>Convergence problems, increasing smallest site-fraction from 1.00E-30 to hardware precision 2.00E-14. You can restore using SET-NUMERICAL-LIMITS</pre> <p>The smallest site fraction in the current POLY3 workspace is automatically increased from the default value 1.00E-30 to the hardware-dependent precision (under Linux, as 2.00E-14). For other subsequent POLY-module calculation in the current TC run, you can use the POLY command <a href="#">SET_NUMERICAL_LIMITS on page 168</a> to restore or reset the smallest site fraction to the previous or another preferred value, as well as to reset other numerical limits.</p>
STEP_AND_MAP (the default)	<p>Settings for MAP and STEP:</p> <pre>GLOBAL TEST INTERVAL /0/: &lt;INTEGER NUMBER&gt;</pre> <p>Settings for MAP:</p> <pre>AUTOMATICALLY ADD INITIAL EQUILIBRIA /Y/: &lt;Y OR N&gt; NUMBER OF MESH ALONG AN AXIS /3/: &lt;INTEGER NUMBER&gt; USE INSIDE MESHING POINTS /N/: &lt;Y OR N&gt; GLOBAL TEST INTERVAL /0/: &lt;INTEGER NUMBER&gt;</pre> <p>The integer number determines how often the Global Minimization should be used during STEP_WITH_OPTIONS and MAP calculations. If it is set to 0 (zero), the recommended global test interval is used: i.e. every tenth step and at each phase change during STEP calculations, and only at node points during MAP calculations. Any other positive integer number, n, suggests it performs a Global Minimization test at every <i>n</i>-th step during STEP and MAP calculations. Of course, the Global Minimization test is always carried out at a phase change or a node</p>

Syntax	ADVANCED_OPTIONS
	<p>point. The Thermo-Calc software is installed with 0 (zero) as the default value, but such a configuration for the default value can be changed by using SET_TC_OPTIONS in the SYS module.</p> <p>AUTOMATICALLY ADD INITIAL EQUILIBRIA /Y/: &lt;Y OR N&gt;</p> <p>When <a href="#">ADD_INITIAL_EQUILIBRIUM</a> on page 119 is not used before MAP, a mesh of initial equilibrium points are added before the mapping itself takes place. This mesh is only available when two (2) axes are already defined. The default on start-up may be changed by SET_TC_OPTIONS in the SYS monitor.</p> <p>NUMBER OF MESH ALONG AN AXIS /3/: &lt;INTEGER NUMBER&gt;</p> <p>An integer for how many intervals of initial equilibrium points to be added along an edge in the diagram. For example, if set to 2 (two), initial equilibrium points are added at the beginning, centre, and end of each axis-variable forming 2 intervals.</p> <p>USE INSIDE MESHING POINTS /N/: &lt;Y OR N&gt;</p> <p>If <b>N</b> the INITIAL_EQUILIBRIUM mesh consists of initial equilibrium points added only along the edge/border of the diagram defined by the axis-variables. If <b>Y</b>, the initial equilibrium points added are also added inside edge.</p>
EQUILIBRIUM_CALCUL	<p>The following prompts affect the ways how the POLY optimization does the Ordinary POLY Minimization to reach the minimum of an equilibrium state.</p> <p>Settings for the minimization of an equilibria:</p> <p>FORCE POSITIVE DEFINITE PHASE HESSIAN /Y/: &lt;Y OR N&gt;</p> <p>CONTROL STEPSIZE DURING MINIMIZATION /Y/: &lt;Y OR N&gt;</p> <p>FORCE POSITIVE DEFINITE PHASE HESSIAN /Y/: &lt;Y OR N&gt;</p> <p>Choose <b>Y</b> or <b>N</b> to determine how to reach the minimum of an equilibrium state in a normal POLY optimization procedure. This is related to the special quantity, the phase stability function QF (phase), for all kinds of phases in an equilibrium state [A phase stability function for a phase is negative when the phase composition is inside a spinodal, and positive everywhere else].</p> <p>If the composition of a solution phase is inside its spinodal, the enforcement of positive definite eigenvalues of a Hessian matrix (i.e. by answering <b>Y</b>) makes the step be taken towards the minima rather than the local maxima. Furthermore, if an eigenvalue (for a phase) of the Hessian matrix is near 0.0, the step-size is large and the answering <b>Y</b> sets a lower limit to this eigenvalue, and reduces the step-size and improves the convergence. The POLY command-sequence SHOW_VALUE QF(phase) shows the size of the lowest eigenvalue of a phase in an equilibrium state.</p>

Syntax	ADVANCED_OPTIONS
	<p>By answering <b>Y</b> it might help the Ordinary POLY Minimization to converge, if there is such a problem, especially if <math>QF(\text{phase})=0</math> for phases.</p> <p>By answering <b>N</b> the Ordinary POLY Minimization routine is applied.</p> <p>For each phase in a defined system, the molar Gibbs energy of the phase is a function of the temperature-pressure condition and its composition:</p> $G_m(X) = G_m(T, P; y_1, y_2, \dots, y_n)$ <p>Compute a Hessian matrix as which describes the curvature of the Gibbs energy curve of this phase at the defined composition X:</p> $\partial^2 G_m / \partial y_i \partial y_j$ <p>Diagonalise this matrix and call the Eigenvalues as <math>e_1, e_2, \dots, e_n</math>. The <math>QF(\text{phase})</math> quantity for this phase is the lowest of these eigenvalues divided by the same values for a corresponding ideal (stoichiometric) phase:</p> $QF(ph) = \min(\{e_1, e_2, \dots, e_n\}) / \min(\{se_1, se_2, \dots, se_n\})$ <p>Here, <math>se_1, se_2, \dots, se_n</math> are the eigenvalues for the ideal phase. Therefore, for an ideal (stoichiometric) phase, the <math>QF(\text{phase})</math> should always be 1.0.</p> <p>CONTROL STEPSIZE DURING MINIMIZATION /Y/: &lt;Y OR N&gt;</p> <p>Choose <b>Y</b> or <b>N</b> to determine whether to introduce a control of step-size while reaching the minimum of an equilibrium state in a normal POLY optimization procedure. By answering <b>Y</b> it might help the POLY optimization to converge, especially if when some site fractions are less than 1E-4.</p>
GLOBAL_MINIMIZATION	<p>The following prompts affect how the Global Minimization is done. Settings for global minimization:</p> <p>USE GLOBAL MINIMIZATION AS MUCH AS POSSIBLE /Y/: &lt;Y OR N&gt;</p> <p>USE GLOBAL MINIMIZATION FOR TEST ONLY? /N/: &lt;Y OR N&gt;</p> <p>MAXIMUM NUMBER OF GRIDPOINTS PER PHASE /2000/: &lt;INTEGER NUMBER&gt;</p> <p>USE GLOBAL MINIMIZATION AS MUCH AS POSSIBLE /Y/: &lt;Y OR N&gt;</p> <p>Choose <b>Y</b> or <b>N</b> to decide if using the Global Minimization Technique from start of calculation or not. The default value on start-up may be changed by SET_TC_OPTIONS in the SYS module.</p> <p>If <b>Y</b> the calculation is done when possible (depending on the condition settings), and a Global Minimization test is always performed when an equilibrium is</p>

Syntax	ADVANCED_OPTIONS
	<p>reached. This costs more computer time but the calculations are more accurate.</p> <p>If <b>N</b> the calculation is not used to reach the equilibrium state. Use <code>global minimization for test only?</code> determines if the Global Minimization test is made against the calculated equilibrium states obtained by the Ordinary POLY Minimization calculation.</p> <p><code>USE GLOBAL MINIMIZATION FOR TEST ONLY? /N/: &lt;Y OR N&gt;</code></p> <p>If <b>Y</b> a calculated equilibrium state obtained by the Ordinary POLY Minimization calculation is tested against the Global Minimization Technique after it is reached; and if found it as unstable, there is an error message.</p> <p>If <b>N</b> the Global Minimization Technique is never tested for or done for all sequential calculations throughout the current TCC run. This implies that Global Minimization Technique is permanently turned off, and that consequently only the Ordinary POLY Minimization routine is used.</p> <p><code>MAXIMUM NUMBER OF GRIDPOINTS PER PHASE /2000/: &lt;INTEGER NUMBER&gt;</code></p> <p>Specify the maximum number of grid points that are computed for each of the phases in the currently defined system, during the calculations enforced by the global minimization. More grid points give a higher robustness and take more computation time. The total number of computed grid points in all phases is limited to <code>2E6</code>.</p>
<code>IGNORE_COMPOSITION_SET_ORDER</code>	<p><code>IGNORE COMPOSITION SET ORDER /N/</code></p>
<code>NEW_COMPOSITION_SET</code>	<p>The following prompts are to specify the additional composition set(s) to handle possible miscibility gap(s) of a certain solution phase:</p> <p><code>PHASE WITH MISCIBILITY GAP: &lt;NAME OF A PHASE&gt;</code></p> <p>Specify the name of the phase with miscibility gap.</p> <p><code>NEW HIGHEST COMPOSITION SET NUMBER /2/: &lt;#&gt;</code></p> <p>The default value is usually one higher than the current value. Each phase has initially one composition set. If a lower value is given, composition sets are deleted. You cannot take away the first composition set.</p> <p>A message displays to show that you need to specify the composition for the composition set # (2,3,...).</p> <p><code>MAJOR CONSTITUENT(S) FOR SUBLATTICE 1: /XX/: &lt;YY&gt;</code></p> <p>The major constituents (<b>YY</b>) in each sublattice can be given. This may simplify giving start values when calculating the equilibrium as phases with miscibility gaps</p>

Syntax	ADVANCED_OPTIONS
	<p>should have different major constituents for each composition set.</p> <p>This prompt is repeated for each sublattice in the phase, sometimes even for all sublattices in the first composition set if such major constituents have not been specified.</p>
MAJOR_ CONSTITUENT	<p>The following prompts are to specify the major constituent(s) on each of the sublattice sites for a composition set of a certain solution phase:</p> <p>PHASE NAME: &lt;NAME OF A PHASE&gt;</p> <p>Specify the name of the solution phase with a new set of major constituents.</p> <p>COMPOSITION SET NUMBER /1/: &lt;#&gt;</p> <p>The default value for the composition set number (#) is usually /1/ as the other composition sets are given major constituents when creating them. Each phase has initially one composition set.</p> <p>MAJOR CONSTITUENT(S) FOR SUBLATTICE 1: /XX/: &lt;YY&gt;</p> <p>The major constituents (YY) on each sublattice of a solution phase can be given. This may simplify giving start values when calculating the equilibrium as phases with miscibility gaps should have different major constituents for each composition set.</p> <p>This question is repeated for each sublattice in the phase.</p>
PHASE_ADDITION	<p>The following prompts are to specify the additional energy term (always being a constant) of a given phase.</p> <p>PHASE NAME: &lt;NAME OF A PHASE&gt;</p> <p>Specify the name of the (stoichiometric or solution) phase with the addition.</p> <p>ADDITION TO G PER MOLE FORMULA UNIT: &lt;XXXXXX&gt;</p> <p>The value (xxxxxx) given is added to the Gibbs energy of the (stoichiometric or solution) phase. It can represent a nucleation barrier, surface tension, elastic energy or whatsoever.</p> <p><input checked="" type="checkbox"/> It is not composition-, temperature- or pressure-dependent.</p>
LIST_PHASE_ ADDITION	No additional prompt.
PRESENT_PHASE	Specify the name of the present phase a the name of the phase that should be present at all calculated equilibria:

Syntax	ADVANCED_OPTIONS
	<p>PRESENT PHASE:</p> <p>PHASE NAME: &lt;NAME OF A PHASE&gt;</p>
T-ZERO TEMPERATURE	<p>NAME OF FIRST PHASE: &lt;PHASE A&gt;</p> <p>NAME OF SECOND PHASE: &lt;PHASE B&gt;</p> <p>The names of phases A and B must be given, for which the T0 temperature (where the Gibbs energies are equal) is to be calculated.</p> <p>If the T0 temperature between the two specified phases is successfully calculated, a message displays, e.g.</p> <p>THE T0 TEMPERATURE IS 840.82 K. NOTE: LIST-EQUILIBRIUM IS NOT RELEVANT</p> <p>The first message shows the calculated T0 temperature between the two specified phases.</p> <p>The second message indicates that after this option calculation with LIST_EQUILIBRIUM is irrelevant and does not list the equilibrium for the system at the T0-temperature.</p>
PARAEQUILIBRIUM	<p>NAME OF FIRST PHASE: &lt;PHASE A&gt;</p> <p>NAME OF SECOND PHASE: &lt;PHASE B&gt;</p> <p>The names of the two target phases A and B, between which the paraequilibrium state is to be calculated, must be entered subsequently or on the same (first) line at once then separated by an empty space, e.g. FCC#1 BCC or FCC#2 M23C6.</p> <p> You need to understand what you are dealing with in terms of calculating a paraequilibrium state between the two specified phases.</p> <p>Specifically, there are four distinguished cases to understand: (1) both chosen phases must have similar interstitial/vacancy sublattices where the fast-diffusion interstitial component(s) occupy; (2) the choice on the target phase pair must be reasonable for the defined system and specified initial overall composition; (3) both target phases should have phase constitution definitions that cover all the defined substitutional and interstitial components of the current alloy system; or (4) it is impossible to calculate the paraequilibrium state between the target phase pairs with given interstitial component(s) in the currently defined system.</p> <p>FAST DIFFUSING COMPONENT: /C/: &lt;INTERSTITIAL COMPONENT (S)&gt;</p> <p>FAST DIFFUSING COMPONENT: /NONE/: &lt;INTERSTITIAL COMPONENT (S)&gt;</p> <p>The name(s) of the fast-diffusing component(s) (C as the default single</p>

Syntax	ADVANCED_OPTIONS
	<p>component) must be given at the above prompts subsequently or at the same (first) prompt. It is possible to specify more than one interstitial component as fast diffusion species.</p> <p>Note the following:</p> <p>Such specified interstitial component(s) must be appropriately defined according to the phase constitution definitions of the two selected phases: these must be located on the interstitial/vacancy sublattices in both chosen phases;</p> <p>If there is only one fast-diffusing component which is carbon, press the &lt;Enter&gt; key to accept the default input at the first prompt; if the single fast-diffusing component is another element (e.g. N), type its name at the first prompt;</p> <p>If there are two or more fast-diffusing components (e.g. C and N), type their names at the above prompts subsequently or at the same (first) prompt (separated by an empty space, such as C N);</p> <p>To finish the input of fast-diffusing elements, accept NONE at a repeated prompt, i.e. by pressing &lt;Enter&gt; key to start the paraequilibrium point calculation;</p> <p>If NONE or a non-existing component name is typed at the first prompt, it means no back diffusion is to be considered, and the para-equilibrium calculation is thus cancelled entirely.</p> <p>If the paraequilibrium state between the two specified phases is successfully calculated, the messages displays e.g.</p> <pre>NP(FCC) = 0.3586 with U-fractions C = 2.71821E-02  N = 4.1548129E-03 NP(BCC) = 0.6414 with U-fractions C = 7.10061E-04  N = 2.3781027E-04 All other compositions the same in both phases Note: LIST-EQUILIBRIUM is not relevant</pre> <p>The first and second lines list the phase amounts expressed in mole-percent [NP (phase)] and the contents of the interstitial components C and N in a specific phase expressed in the so-called u-fractions [u-f(phase,C) and u-f(phase,N)], for the phase A (in this case as FCC) and phase B (in this case as BCC), respectively. The third line states that the compositions of the matrix component and all the remaining compositions (regarding substitutional components) in both the target phase A and target phase B are the same at the current paraequilibrium state, while these are not shown on screen. The last line indicates that after this advanced-option calculation the LIST_EQUILIBRIUM command is irrelevant and does not list the paraequilibrium state for the system at the current condition.</p>

Syntax	ADVANCED_OPTIONS
	<p>However, if the single-point calculation of the paraequilibrium state between the two specified phases has failed, these messages display:</p> <pre>*** ERROR      4 IN NS01AD *** NUMERICAL ERROR</pre> <p>This implies that the chosen target phase pair may be unreasonable for the defined alloy system or for the defined initial overall composition, or one or both phases may have inappropriate phase constitution definitions regarding the specified interstitial component(s). Then, you must either modify the settings of initial overall composition or specify the reasonable target phase pair with an appropriate choice of the fast diffusion interstitials in the defined alloy system.</p>
STABILITY_CHECK	<pre>STABILITY CHECK ON? /Y/: &lt;Y OR N&gt;</pre> <p>The default is <b>Y</b> to switch on the automatic stability check during all subsequent single-point equilibrium and MAP/STEP calculations. By answering <b>N</b>, there is no stability check in various calculations.</p> <pre>CHECK ALSO FOR UNSTABLE PHASES? /Y/: &lt;Y OR N&gt;</pre> <p>If the automatic stability-check option is switched on choose to also check the stability for unstable phases. The default is <b>Y</b> and if an unstable phase is found to be located in a miscibility gap during a subsequent single-point equilibrium or MAP/STEP calculation, a warning message informs you to selectively make adjustments in the calculation settings [e.g. suspending the unstable phase, or using FORCED automatic start values for phase constituents by the <b>S_A_S_V F</b> command-sequence, or creating other composition sets, etc.]. By answering <b>N</b> the stability check is enforced only to stable phases in the system.</p>
TOGGLE_ALTERNATE_MODE	<pre>SET ALTERNATE TOGGLE TO DEFAULT, ALWAYS, OR NEVER? SET GLOBAL TOGGLE TO DEFAULT, ALWAYS, OR NEVER?</pre> <p><b>DEFAULT</b> means that the experiment points are calculated according to the Alternate Technique depending on the <b>SET_ALTERNATE</b> command.</p> <p><b>ALWAYS</b> means the experiment points are always calculated according to the Alternate Technique even if the Alternate Mode is switched off in the PARROT module.</p> <p><b>NEVER</b> means the experiment points are calculated as normal equilibria even if you <b>SET_ALTERNATE</b> in the PARROT module.</p>
SHOW_FOR_T=	<pre>TEMPERATURE (K) /298.15/: &lt;TEMPERATURE_IN_K&gt;</pre> <p>Specify the new temperature condition (in K) under which the values of some specific state variable(s) or derived/partial variable(s) or defined symbol(s) for</p>



Syntax	ADVANCED_OPTIONS
	<p>various thermodynamic properties of the entire system, of components, or of phases) in the currently-defined system (being in a <i>frozen</i> state) is shown on screen.</p> <p>STATE VARIABLE OR SYMBOL /VM/: &lt;STATE VARIABLE OR SYMBOL NAME(S)&gt;</p> <p>Specify the name(s) of the desired state variable(s) or derived/partial variable(s) or defined symbol(s) for various thermodynamic properties of the entire system, of components, or of phases) in the currently-defined system. More than one state variable or symbol of interest can be simultaneously specified on the same line. For example, you can choose to show the values of VM or GM (i.e. molar volume or molar Gibbs energy of the entire system), or of VM(*) or HM(*)<sub>T</sub> (i.e. molar volumes or isobaric heat capacity of all phases), or of ACR(*), DGM(*) and LNACR(*,FCC) [i.e. activities of all system components, driving forces for all phases, and activities (in logarithm) of all system components in the FCC solution phase], under the new temperature condition (being in a frozen state).</p>
OUTPUT FILE FOR SHOW	A window opens with a default name for the file <code>tc_show.dat</code> . Choose a location to save the file and click Open.

## AMEND\_STORED\_EQUILIBRIA

This command gives information about the calculated blocks (and phase regions included in blocks) after the STEP or MAP calculation(s). It allows you to list all or part of the calculation results, to suspend all or parts of the calculation results that are redundant or where metastable equilibria are calculated, and to restore all or parts of the calculation results (if having been suspended by another AMEND\_STORED\_EQUILIBRIA command).

The workspace for storing equilibria may overflow during stepping or mapping, and is then written to a file as blocks. Each block usually contains one or more ranges of equilibrium regions.

Use one these options:

- **L** to list the calculated equilibria (all or a specified block)
- **S** to suspend everything (all blocks and their regions)
- **Q** to suspend each set of equilibria individually (specified blocks and/or regions)
- **R** to restore everything (all blocks and their regions)

Syntax	AMEND_STORED_EQUILIBRIA
Prompts	<p>NAME: &lt;NAME OF A DEFINED TABLE&gt;</p> <p>List (L) the calculated equilibria, suspend everything (S) or suspend each set of equilibria individually (Q), or restore everything (R).</p>
	<p>BLOCK /*/: &lt;BLOCK NUMBER&gt;</p> <p>Specify a block number in the option L, S, Q or R. Or include all the blocks in the amending option, by accepting the wildcard * (press &lt;Enter&gt;).</p> <p>For L, a block (if a block number is specified) or all the blocks (if the wildcard * is accepted/used), with the regions and the equilibrium details, that are calculated during stepping or mapping is listed on screen or in a textual file.</p> <p>For Q, each ranger in a block (if a block number is specified) or in all blocks (if the wildcard * is accepted/used) then choose:</p>
	<p>S (USPEND) K (EEP) /K/: &lt;S OR K&gt;</p> <p>For S or R, if a block is specified, you are asked what region in the block should be suspended or restored. However, if the wildcard * is accepted/used, you are asked the following:</p> <p>REALLY SUSPEND ALL /N/: &lt;Y OR N&gt;</p> <p>REALLY RESTORE ALL /N/: &lt;Y OR N&gt;</p> <p>If the answer is N, the program asks for which block(s) and which region(s) in a certain block to execute the S or R action.</p> <p>REALLY SUSPEND ALL /N/: &lt;Y OR N&gt;</p> <p>Y suspends everything.</p> <p>REALLY RESTORE ALL /N/: &lt;Y OR N&gt;</p> <p>Y restore everything.</p>
	<p>RANGE: &lt;RANGE(S) OF REGION&gt;</p> <p>Specify one or more ranges to be suspended (the S option) or restored (the R option). The wildcard * suspends or restores all ranges in the specified block.</p> <p>In order to know the ranges the LIST option must first be used.</p>
	<p>S (USPEND) K (EEP) /K/: &lt;S OR K&gt;</p> <p>The Query suspend option (Q) asks for each region in a certain block if it should be suspended or kept. Suspended regions are not included on sequentially generated plots.</p>
	<p>OUTPUT FILE: /SCREEN/: &lt;FILE NAME&gt;</p>

Syntax	AMEND_STORED_EQUILIBRIA
	This prompt is only for listing (the <code>L</code> option), and after it the command is terminated. The file name must be given here; or accept the default <code>SCREEN</code> (terminal) by pressing <Enter>. A list of stored equilibria as various blocks (with all their ranges) are shown out on screen or the file.

## CHANGE\_STATUS

In the POLY module, set the status for components, species and phases in the defined system for all the sequential calculations (single-point, stepping and mapping) in equilibrium or local/partial equilibrium state. Each component, species and phase has a status. The default status is `ENTERED`.

The most important use is to calculate metastable equilibria and metastable phase diagrams by setting some phases (that would otherwise be stable) to the `SUSPENDED` or `DORMANT` phase-status. Another important applications is to calculate paraequilibria by setting some components to the `SPECIAL` component-status.

For a component and for a species, the status can be one of the following:



- `ENTERED` - the component(s) or species are included in the calculation. This is the default status.
- `SUSPENDED` - the component(s) or species are not considered in the calculation.
- `SPECIAL` means - specified component(s) are not included in summations for mole or mass fractions. It only works for component(s).



Only component(s) can have the status `SPECIAL`, which implies that these are not included in summations for mole or mass fractions.

For example, for the *u-fractions* or other normalized fractions, when one or more of the components are excluded from the summation, you must specify which component(s) should be excluded from the calculation of mole or mass fraction. This component status is particularly useful when calculating paraequilibrium states. Such component(s) are normally interstitial component, and must have the status `SPECIAL`. This is assigned by the `CHANGE_STATUS` command.

Syntax	CHANGE_STATUS
Prompts	FOR PHASES, SPECIES OR COMPONENTS? /PHASES/: <KEYWORD> Keyword = phase or species or components
	PHASE NAME(S) : <NAME(S) OF THE PHASE(S)>  For <code>phase</code> as the keyword, the names of the phases that have their status changed must be given (all on one line). A comma or space must be used as separator. The status to be

Syntax	CHANGE_STATUS
	<p>assigned to the phases can also be given on the same line if preceded with an equal sign =.</p> <p> An asterisk, *, can be used to denote all phases. The special notations *S, i.e. a wildcard * directly followed by an S, sign, means all suspended phases. In the same way, *D means all dormant phases, and *E means all entered phases.</p>
	<p>NAME(S) : &lt;NAME(S) OF THE SPECIE(S) OR COMPONENT(S)&gt;</p> <p>For <code>species</code> or <code>component</code> as the keyword, the names of the species or components that have their status changed must be given (all on one line). A comma or space must be used as separator. Similarly to the case of <code>phase</code> as the keyword, the status to be assigned to the species or components can also be given on the same line if preceded with an equal sign =.</p> <p> An asterisk, *, can be used to denote all species or components. The special notations *S, i.e. a wildcard * directly followed by an S, sign, means all suspended species or components. In the same way, *E means all entered species or components.</p>
	<p>STATUS /ENTERED/: &lt;NEW STATUS&gt;</p> <p>The new status to be assigned must be given.</p> <p>For <code>species</code>, the values <code>ENTERED</code> or <code>SUSPENDED</code> can be used.</p> <p>For <code>components</code>, the status <code>ENTERED</code>, <code>SUSPENDED</code> or <code>SPECIAL</code> can be given. <code>SPECIAL</code> means that this component is excluded from sums for mole fractions and mass fractions, which is useful when calculating the <i>ufractions</i> or other normalized fractions of system components.</p> <p>For <code>phases</code>, the status <code>ENTERED</code>, <code>SUSPENDED</code>, <code>DORMANT</code> or <code>FIXED</code> can be given. <code>DORMANT</code> means the same as suspended but the driving force is calculated. <code>FIXED</code> means that it is a condition that the phase is stable at a certain amount.</p> <p>For example, for the <i>ufractions</i>, when one or more of the components are excluded from the summation, you must specify which component should be excluded from the calculation of the mole fraction. This component must have the status <code>SPECIAL</code>. This is assigned by the <code>CHANGE_STATUS</code> command: <code>Change_Status comp C=special.</code></p>
	<p>START VALUE, NUMBER OF MOLES /0/: &lt;INITIAL AMOUNT&gt;</p> <p>For <code>ENTERED</code> phases, an <code>initial amount</code> of the phase can be given. Normally, 0 is given if the phase is not likely to be stable, and 0.5 or 1 or any positive number if the</p>

Syntax	CHANGE_STATUS
	<p>phase could be stable, but such an initial amount is only used as the rough starting estimation in the equilibrium calculations.</p>
	<p>NUMBER OF MOLES /0/: &lt;EQUILIBRIUM AMOUNT&gt;</p> <p>For FIXED phases, the <code>equilibrium</code> amount of the phase [always using an initial estimation being the <code>NPF(phase)</code> value which it is the normalized mole number of components (per mole formula unit) of the specific status-fixed phase] must be given. If the equilibrium amount is zero, then the phase is at its stability limit.</p> <p>Special attentions should be paid when specifying a FIXED phase status in equilibrium calculations (for single points, stepping or mapping calculations), as described below:</p> <p>The phase amount variables, <code>NP(phase)</code>, <code>BP(phase)</code> and <code>VP(phase)</code>, as well as all their M/W/V-suffixed quantities, should not be used as conditions. Instead, use the <code>CHANGE_STATUS</code> command to set a relevant condition, e.g. <code>CHANGE_STATUS phase &lt;phase&gt;=fix &lt;amount&gt;</code> where the fixed <code>&lt;amount&gt;</code> is roughly the same as the F-suffixed quantity <code>NPF(phase)</code>.</p> <p>The <code>NPF(phase)</code> quantity is the normalized mole number of components (per mole formula unit) of the specific phase in the defined system, which unlike other F-suffixed state variables [e.g. <code>GF(phase)</code>, <code>HF(phase)</code> and <code>DGF(phase)</code>] cannot be directly applied in any <code>POLY</code> command, implying that it cannot be directly evaluated or listed/shown. If intended to shown such a normalized phase amount value in an equilibrium state, you should use a properly-entered symbol (function or variable), for example: <code>NPFabc = NP(abc)/NA</code> or <code>NPFabc = NPM(abc)/NA*N</code>. <code>N</code> is the total system size (in mole). The <code>NA</code> value is a quantity that is phase-dependent (and sometimes also equilibrium-dependent for ionic solution phases), and is the total atomic number in a mole-formula-unit of the specific phase <code>abc</code> (excluding interstitial component and, of course, vacancy). For example, the <code>SIGMA</code>, <code>FCC</code>, <code>BCC</code> and <code>LIQUID</code> phases (among others) in a defined Fe-Cr-Ni-C-N-O system (retrieved from a specific database) may be modelled by certain models, and their <code>NA</code> values must be evaluated in different ways, as described below:</p> <pre>LIQUID (C,Cr,CrO3/2,Fe,FeO,FeO3/2,N,Ni,NiO)1 → NA = 1 FCC_A1 (Cr,Fe,Ni)1(Va,C,N,O)1 → NA = 1 BCC_A2 (Cr,Fe,Ni)1(Va,C,N,O)3 → NA = 1 SIGMA (Fe,Ni)8(Cr)4(Cr,Fe,Ni)18 → NA = 30</pre> <p>If in the same Fe-Cr-Ni-C-N-O system the liquid solution phase is modelled by the Two-Sublattice Ionic Liquid Model, i.e.:</p> <pre>IONIC_LIQ (Cr+3,Fe+2,Ni+2)p(VA,C,N,O-2,FeO3/2)q,7</pre> <p>then the evaluation of its <code>NA</code> value becomes even more complicated:</p> $NA = p + q*y_{C2} + q*y_{N2} + q*y_{O2} + q*y_{FeO2} + q*y_{FeO3/2}$

Syntax	CHANGE_STATUS
	<p>where the stoichiometric coefficients <math>p</math> and <math>q</math> are also dependent upon the real equilibrium state (rather than having fixed values in the system). Similar situations occur for other (solid) phases which are described by a multiple sublattice model with ionic constituents, such as SPINEL and HALITE phases in some databases.</p> <p>There is no strange thing when using a zero value [i.e. 0] in a FIXED phase-status, since it means the specified phase is stable in equilibrium state but has a zero-amount of mass in the equilibrium calculations; in other words, on a phase diagram, the specific phase is on a zero-fraction line (ZFL), i.e. it starts becoming stable on one side of a corresponding phase-boundary line or unstable on the other side of the same boundary. It is often and efficient to do so when calculating e.g. solidus equilibrium states.</p> <p>However, when a non-zero value [it must always be positive; e.g. 1 or 0.5 or 0.3 or 1.5] is to be specified in a FIXED phase-status, it is unnecessarily the exactly same stable amount of the specific FIXED-status phase in a calculated equilibrium state any longer; instead, the &lt;equilibrium amount&gt; value is the NPF(phase) value that is only roughly used as the estimated starting-value of the FIXED-status phase in the equilibrium calculations.</p> <p>Therefore, a FIXED-status for a liquid phase being unity does not necessarily imply that it is a liquidus equilibrium state (where the liquid phase is in equilibrium with some solid phases but the liquid phase takes all the mass in the defined system). A unity value for setting the liquid phase status in calculating liquidus equilibrium state can only be used when the liquid mixture phase is predefined as a single-sublattice solution phase (such as metallic liquid phase in multicomponent alloy systems) and the total system size as one mole (i.e. <math>N=1</math>).</p> <p>When a phase is described by a solution model in which two or more sublattices are considered and these sublattice sites may also have different stoichiometric coefficients [meaning that the mixture phase could have more than one atom in formula <math>[NA&gt;1]</math>; see some examples above], the unity value should not be used when setting the FIXED status for the phase; instead, you should use an appropriate value that ranges from 0 to a NPF (phase) value that equals to or is smaller than <math>1/NA</math> (if the total system size <math>N=1</math>) or <math>1/NA*N</math> (if <math>N</math> differs from unity). For this reason, if a multicomponent system bears an IONIC_LIQUID phase that is described by the Two-Sublattice Ionic Liquid Model (or any other multiple-sublattice ionic solution phases), it is difficult to use a proper NPF (ION_LIQ) value in setting its FIXED phase-status, because that should be less than (or equal to) the complex value of</p> $N/[p + q*Y_{C2} + q*Y_{N2} + q*Y_{O22} + q*Y_{FeO2\ 3/2}].$

## Examples

For example, to obtain the metallic fraction in a system with carbon as an interstitial component, you can set the component status for carbon as SPECIAL:

---

Change\_status comp C=special



The `SUSPENDED` status for components and species does not always work as expected.

For a phase, it may have one of these statuses:

- `ENTERED` - the phase(s) are included in the equilibrium calculations and these are stable if that minimizes the total Gibbs energy in the defined system. This is the default status for all phases already retrieved from the chosen database(s). An `ENTERED` phase-status is always associated with an initially-estimated amount [in mole number; normally, as 0 if the phase is not likely to be stable, and as 0.5 or 1 or any positive number if the phase could be stable] but it is only used as the rough starting value in the equilibrium calculations.
- `SUSPENDED` - the phase(s) are not considered in the equilibrium calculations.
- `DORMANT` - the phase(s) are not considered in the equilibrium calculations but their driving forces for precipitation are calculated.
- `FIXED` - it is an equilibrium condition that the status-fixed phase must be stable, and be in equilibrium at a specified amount [always using an initial estimation being the `NPF (phase)` value which it is the normalized mole number of components (per mole formula unit) of the specific status-fixed phase]. See more descriptions at the end of this command.

## COMPUTE\_EQUILIBRIUM

The full equilibrium state is calculated for the given set of conditions. The Global Minimization Technique is by default enforced in this command (`C_E`), while it can be disabled temporarily (for the current single-point equilibrium calculation) if using `C_E –` or `C_E *` command-combination, or permanently (for all the sub sequential single-point calculations or stepping/mapping calculations within the current TCC run) if having decisively switched it off by a user (or possibly in some special modules) through changing the minimization option using the [ADVANCED\\_OPTIONS on page 125](#) → `MINIMIZATION_OPTION` command-sequence.

Syntax	COMPUTE_EQUILIBRIUM
Prompt	<p>The C_E command can be used, in order to enforce the ordinary POLY minimization routines in an equilibrium calculation; this is because of that the ordinary C_E command is now associated with the Global Minimization Technique, and only after the Global Minimization</p> <p>If technique is permanently switched off the C_E command makes no difference from the C_E – command-combination.</p> <p>Only certain types of equilibrium conditions [e.g. T, P, N, N(&lt;component&gt;), X (&lt;component&gt;), B, B(&lt;component&gt;), and W(&lt;component&gt;)] are fully supported in the Global Minimization mode (called <i>Direct Global Minimization</i>); and when other types of equilibrium conditions are used, after the initial POLY, a Global Minimization test and corrections are performed until the lowest minimum is found (called <i>Indirect Global Minimization</i>).</p> <p>If there is any problem with convergence, you may try the C_E * command-combination. The character * enforces the command to use an advanced technique to obtain a complex equilibrium. However, after a successful C_E * calculation, you may repeat the C_E command and can check the status of phases, species or components (with <a href="#">LIST_STATUS on page 157</a> → CPS command-sequence) and equilibrium conditions (with <a href="#">LIST_CONDITIONS on page 155</a>) and list out the calculation results (with <a href="#">LIST_EQUILIBRIUM on page 156</a>), because such actions may tell you how to further modify various settings for your current calculation. This command-combination is not that useful anymore, because the Global Minimization Technique that is always associated with the C_E command is even more powerful and more precise in finding the most-stable equilibrium state in a complex heterogeneous interaction system; therefore, the C_E * command-combination is functional and can be used only after the Global Minimization mode has already been disabled temporarily or permanently.</p> <p>Some phases that are not stable in the current equilibrium state may not have their most favourable composition after this command, and thus their driving forces may not be correct. You can force the program to correctly calculate the driving forces of metastable phases, by giving repeated C_E commands until the number of iterations (that is shown on screen after this command) is reduced to 2.</p> <ul style="list-style-type: none"> <li><input checked="" type="checkbox"/> Also see the POLY command <a href="#">SET_NUMERICAL_LIMITS on page 168</a> which can set the approximate driving force for metastable phases option on or off in all the subsequent POLY calculations within the current TCC run.</li> <li><input checked="" type="checkbox"/> If an equilibrium state for the defined system is not found, an error message is given.</li> </ul>



Syntax	COMPUTE_EQUILIBRIUM
	You can try repeating this command a few times, or change some of settings for the numerical limits, for starting variables and starting values, for starting constitutions of certain phases and for reference states of certain components, or to verify some of the defined conditions.

## COMPUTE\_TRANSITION

This command is a combination of the `CHANGE_STATUS`, `SET_CONDITION` and `COMPUTE_EQUILIBRIUM` commands. It allows a direct calculation when a new phase may form by varying one of the already-set conditions. It can be used only after at least one equilibrium is calculated successfully; otherwise, you are informed on the necessity of first making an equilibrium calculation to find out the stable phases under the current conditions.

When this command is used, the program calls the command [CHANGE\\_STATUS on page 59](#) to temporarily change the phase status of a specified phase as `FIXED` at the *zero* amount, and at the same time to temporarily release one of the existing equilibrium conditions (which is chosen by you). The program calculates a new equilibrium in which that specific phase is stable but its equilibrium amount in the system is zero. The released condition is then assigned with a calculated value that ensures the calculated equilibrium. Afterwards, the program automatically changes the phase status of that specific phase back to `ENTERED`, and resets the temporarily released condition as one of the conditions and assigns it with the value that is calculated to ensure the zero-amount formation of that specific phase.

This command is useful to find melting temperature, boiling temperature, or solubility limits, and generally when you want to set the most optimal conditions for calculating an equilibrium where a specific phase becomes stable. It can also be used when you want to know exactly how far away the defined conditions are from the value that can ensure a zero-amount of a specific phase in the system when other conditions remain the same.


After a successful `COMPUTE_TRANSITION` calculation, you can issue a [COMPUTE\\_EQUILIBRIUM on page 139](#) calculation to assure the calculated transitional equilibrium is a really stable one, and can also use [LIST\\_EQUILIBRIUM on page 156](#) to see the details of transitional equilibrium state.

Syntax	COMPUTE_TRANSITION
Prompts	<p>PHASE TO FORM: &lt;PHASE NAME&gt;</p> <p>A new phase name, e.g. BCC that is expected to form, is specified here. This changes the status of this new phase to be FIXED as 0 amount, and the program shows the information such as:</p> <pre>You must remove one of the these conditions P=100000, T=800, N=1, X(Fe)=.5    DEGREE OF FREEDOM 0</pre> <p>If the key word ANY is used when prompted for Phase to form (instead of a specific phase name), it is possible to find out any new phase to be formed, in a given varying direction sign and at an estimated change of the released condition: a negative sign means at a lower value of the released condition any new phase is to be found, and a positive sign at a higher value; an estimated change of the released condition implies where any new phase is expected (but it is only estimated value, so any value within its reasonable scale would be enough). Such calculations can be repeated if required. This feature is useful to find out all possible phase transformations along a certain released condition.</p>
	<p>GIVE THE STATE VARIABLE TO BE REMOVED /T/: &lt;ONE CONDITION&gt;</p> <p>One condition must be removed, in order to calculate the transition equilibrium where the specified (or any) new phase to be formed at a calculated value of this released variable.</p>
	<p>Therefore, the message may display (after a successful calculation) if, for example, X (Fe) is entered:</p> <pre>To form BCC the condition is set to X(Fe)=.48605791769</pre> <p>This calculated value is assigned as the parameter of that removed condition, in this case, the X (Fe) variable. If the LIST_CONDITIONS command is typed this message displays:</p> <pre>P=100000, T=800, N=1, X(Fe)=4.86057918E-1 DEGREES OF FREEDOM 0</pre> <p>If the key word ANY (instead of a specific phase) is given as the phase name when it is prompted for Phase to form, the line is prompted for a given varying direction sign and an estimated change of the released condition before the calculation of transition equilibrium:</p>
	<p>ESTIMATED CHANGE (WITH SIGN) /1/: &lt;+/-#&gt;</p> <p>A given varying direction sign and an estimated change of the released condition, in this case as X (Fe) , must be given here: a negative sign means at a lower value of the released condition any new phase is to be found, and a positive sign at a higher value; an estimated change of the released condition implies where any new phase is expected (but</p>

Syntax	COMPUTE_TRANSITION
	<p>it is only estimated value, so any value within its reasonable scale would be enough). For example, if a combination of -0.02 is input, this message may display (after a successful calculation):</p> <pre>To form BCC_A2#1 the condition is set to X(Fe)=.493708756187</pre> <p>This calculated value is then assigned as the parameter of that removed condition, in this case, the <code>X(Fe)</code> variable. The message is shown if the <code>LIST_CONDITIONS</code> command is typed:</p> <pre>P=100000, T=800, N=1, X(Fe)=4.93708756E-1 DEGREES OF FREEDOM 0</pre>

## CREATE\_NEW\_EQUILIBRIUM

During data-assessments using the PARROT/ED\_EXP modules, you can, in the POLY module, create several equilibria with different sets of conditions and phases (but normally with the same set of components). By default, there is one equilibrium. To keep the set of conditions and phase for this equilibrium, create another one using this command, and use another set of conditions for that. Two equilibria may be useful to calculate easily the enthalpy difference between two states. In the PARROT module, the experimental information is stored as a sequence of equilibria.

Syntax	CREATE_NEW_EQUILIBRIUM
Prompts	<p>EQUILIBRIUM NUMBER /2/: &lt;A NEW EQUILIBRIUM NUMBER&gt;</p> <p>Each equilibrium in the POLY3 workspace is identified by a unique integer number. Such an equilibrium number can be recalled with <a href="#">SELECT_EQUILIBRIUM</a> on page 162.</p>
	<p>INITIATION CODE /2/:</p> <p>When an equilibrium is created, you can choose to <code>ENTER</code> all components and phases (initiation code 2), <code>ENTER</code> the components only (initiation code 1) or <code>SUSPEND</code> everything (initiation code 0). No other values are legal.</p> <p> The entered components and phases can later be changed with <a href="#">CHANGE_STATUS</a> on page 59.</p>

## DEFINE\_COMPONENTS

Change the set of components. By default, the elements are used as components. The set of components can be important because some conditions are set using components, for example, the amounts, activities or chemical potentials.

For example, in the system Fe-Si-O, you can define FEO, FE2O3 and SIO2 as components, thus replacing the default FE, SI and O.



This implies a command [REINITIATE\\_MODULE](#) on page 161 and it should be given as the first command in the POLY module.

Syntax	DEFINE_COMPONENTS
Prompt	<p>GIVE ALL NEW COMPONENTS /EXISTING COMPONENTS/: &lt;NEW COMPONENTS&gt;</p> <p>The <code>new components</code> must be specified all on one line. These replace the existing component definitions.</p> <p> The number of components cannot be changed with this command. Use <a href="#">CHANGE_STATUS</a> on page 59 instead.</p> <p>To keep some existing components, it is recommended that you also enter these on the line. Otherwise, the added new components may not be defined correctly. This is especially important if some components are built out of several elements.</p> <p> The new components do not have to be present as species.</p>

## DEFINE\_DIAGRAM

This allows automatic calculation and plotting of a diagram with a single command. It is the same as the `DEFINE_MATERIAL` command up to when the first equilibrium is calculated. The alloy `OPTION` feature is also available in this command to specify alloying compositions for a special alloy predefined by the `OPTION` keyword in a selected database (e.g. the TCNI Ni-based Superalloys Database).

Use this command to calculate all types of phase diagrams after specifying all composition value and an initial temperature (if temperature is used as an axis). However, for binary and ternary diagrams, the special `BIN` and `TERN` modules may be preferred.


It then lists all the independent variables for the defined system (i.e. temperature and the components) and asks for a variable as the X-axis. You must also specify a maximum and minimum for the X-axis. The second axis (Y-axis) can be another composition (or the temperature if that is not on the X-axis) from the independent variable list. The program then calculates and plots a *phase diagram*, as there are two independent quantities on the axes.

Alternatively, select a dependent quantity as the Y-axis variable from the second list on screen (e.g. the amount of all phases, composition of a specific phase, or fractions of a component in all phases), and the program calculates and plots how this quantity depends on the condition on the X-axis. This is a *property diagram*.

This command ends up within the POST module monitor. You can refine the calculated phase diagram or property diagram.

Moreover, many more property diagrams with axes other than compositions can also be plotted (after the calculation), using [SET\\_AXIS\\_VARIABLE on page 164](#) in the sequent POST monitor.

Syntax	DEFINE_DIAGRAM
Prompts	<p>These prompts are given:</p> <p>SAME ELEMENTS AS BEFORE /Y/? &lt;Y OR N&gt;</p> <p>MOLE PERCENT OF &lt;ELEMENT&gt; /##/: &lt;VALUE&gt;</p> <p>or</p> <p>MASS PERCENT OF &lt;ELEMENT&gt; /##/: &lt;VALUE&gt;</p> <p>DATABASE /ABCDE/: &lt;DATABASE NAME&gt;</p> <p>MAJOR ELEMENT OR ALLOY: &lt;ELEMENT NAME&gt;</p> <p>COMPOSITION IN MASS (WEIGHT) PERCENT? /Y/: &lt;Y OR N&gt;</p> <p>1ST ALLOYING ELEMENT: &lt;ELEMENT NAME&gt;</p> <p>MASS (WEIGHT) PERCENT: &lt;AMOUNT OF THE ABOVE SPECIFIED ELEMENT&gt;</p> <p>2ND ALLOYING ELEMENT: &lt;ELEMENT NAME&gt;</p> <p>NEXT ALLOYING ELEMENT: &lt;ELEMENT NAME&gt;</p> <p>MASS (WEIGHT) PERCENT: &lt;AMOUNT OF THE ABOVE SPECIFIED ELEMENT&gt;</p> <p>TEMPERATURE (C) /1000/: &lt;TEMPERATURE OF INTEREST IN OC&gt;</p> <p>REJECT PHASE(S) /NONE/: &lt;LIST OF PHASE(S) TO BE REJECTED&gt;</p> <p>RESTORE PHASE(S) /NONE/: &lt;LIST OF PHASE(S) TO BE RESTORED&gt;</p> <p>OK? /Y/: &lt;Y OR N&gt;</p> <p>SHOULD ANY PHASE HAVE A MISCIBILITY GAP CHECK? /N/: &lt;Y OR N&gt;</p> <p>PHASE WITH MISCIBILITY GAP: &lt;PHASE NAME&gt;</p> <p>MAJOR CONSTITUENT(S) FOR SUBLATTICE #: /AA/: &lt;CONSTITUENT(S)&gt;</p> <p>PHASE WITH MISCIBILITY GAP: &lt;PHASE NAME&gt;</p> <p>The first equilibrium is calculated, as with <a href="#">DEFINE_MATERIAL on page 147</a>. Then a list of all independent conditions suitable to be chosen as X/Y-axis variables is given by the program.</p>
	<p>QUIT? /Y/: &lt;Y OR N&gt;</p> <p>This question is asked only when the axis variables are already defined, or if the command DEFINE_DIAGRAM is used. It then offers an opportunity to quit (Y) the calculation or to continue (N) the calculation but by defining other axes.</p>
	<p>GIVE THE NUMBER OF THE CONDITION TO VARY /1/: &lt;A CONDITION INDEX&gt;</p>


Syntax	DEFINE_DIAGRAM
	<p>Select one of the independent conditions by giving its index on the condition list as the X-axis variable.</p>
	<p>MINIMUM VALUE /XXX/: &lt;MINIMUM VALUE FOR X-AXIS&gt;</p> <p>Specify the minimum value of the chosen X-axis variable. A default value is shown automatically by the program; press &lt;Enter&gt; to accept it or input another value.</p>
	<p>MAXIMUM VALUE /YYY/: &lt;MAXIMUM VALUE FOR X-AXIS&gt;</p> <p>Specify the maximum value of the chosen X-axis variable. A default value is shown automatically by the program; press &lt;Enter&gt; to accept it or input another value. Then another list with some dependent quantities is given by the program, which can be selected as the Y-axis variable.</p>
	<p>GIVE THE NUMBER OF THE QUANTITY ON THE SECOND AXIS /#/: &lt;##&gt;</p> <p>Select one of the independent conditions or dependent quantities as the Y-axis variable, by giving its corresponding index given on the condition lists.</p> <div style="border: 1px solid black; background-color: #d4edda; padding: 10px; margin: 10px 0;">  <p>It must be different from the X-axis variable already selected.</p> </div> <p>If selecting one of dependent quantities (by giving the corresponding number from the second list) as the Y-axis, then a property diagram is to be automatically calculated (through a normal stepping procedure) and generated. For composition of a phase the phase name is asked for further specification subsequently.</p> <p>If selecting any of the other independent variables (conditions) on the first list as the Y-axis, then a phase diagram is automatically calculated (through a mapping procedure) and plotted.</p>
	<p>NAME OF PHASE: /ABC/: &lt;PHASE NAME&gt;</p> <p>This is prompted only in case of that the composition of a phase is selected as the Y-axis variable. The phase name for which the composition varied along with X-axis variable should be specified.</p>
	<p>MULTIPLE START POINTS? /Y/: &lt;Y OR N&gt;</p> <p>This question is to confirm whether or not to let the program to automatically generate and use multiple start points for mapping the defined phase diagram.</p>
	<p>SAVE FILE /RESULT/: &lt;FILE NAME&gt;</p> <p>The file name where the calculations are stored (saved as a *.POLY3 file) should be specified; the default file name is RESULT.POLY3 (Windows) or RESULT.poly3 (Linux).</p>


## DEFINE\_MATERIAL

Read data for a system from a database in the POLY module. It is convenient to use for alloys when there is a major component and the amount of the other elements is known in mass (weight) fraction. The command reads the system from the specified database, sets the composition and temperature (and pressure equal to 1 bar) and calculates the equilibrium state before the prompting for a new command. You can list the results with [LIST\\_EQUILIBRIUM on page 156](#) or set a new composition or set axis for a STEP or MAP command.




You cannot append data from different databases in this way. Use this command with data from a USER database.

Syntax	DEFINE_MATERIAL
Prompts	<p>SAME ELEMENTS AS BEFORE /Y/? &lt;Y OR N&gt;</p> <p>This question is asked only if some data is already read from the database, or if the command DEFINE_MATERIAL or DEFINE_DIAGRAM is used. It then offers a convenient way to change the composition and temperature with one command.</p> <p> This command only works properly in cases where the composition of the material system is already defined as in the mole-percent or mass-percent unit.</p>
	<p>MOLE PERCENT OF &lt;ELEMENT&gt; /##/: &lt;VALUE&gt;</p> <p>or</p> <p>MASS PERCENT OF &lt;ELEMENT&gt; /##/: &lt;VALUE&gt;</p> <p>If you have decided to use the same materials system (available in the current POLY3 workspace) by accepting the default answer (Y) to the previous prompt <i>Same elements as before /Y/?</i>, one of the alternative prompts display for each of the components in the defined system, depending on how the composition is defined (either in mole-percent, or in mass-percent).</p> <p>Prompts are repeated until all the defined components are completed. Then, the program prompts to specify the temperature condition.</p>
	<p>DATABASE /ABCDE/: &lt;DATABASE NAME&gt;</p> <p>The database with the description for the material must be given, or press &lt;Enter&gt; if using the current database. It is possible to give a USER database.</p>
	<p>MAJOR ELEMENT OR ALLOY: &lt;ELEMENT NAME&gt;</p> <p>The material must have a major element, usually the element which is present in the largest amount. The fraction of this element is not set but is the rest.</p>

Syntax	DEFINE_MATERIAL
	<p>In some databases there are the alloys predefined. An alloy has a default major element and have limits of the amounts of the alloying elements. If you stay within these limits the calculation gives reasonable results.</p>
	<p>COMPOSITION IN MASS (WEIGHT) PERCENT? /Y/: &lt;Y OR N&gt;</p> <p>The default is that input is taken as mass percent, but it is possible to change to mole percent by answering N.</p> <div>  <p>Composition should be given in PERCENT not FRACTION, as it is required for the <math>w</math> and <math>x</math> state variables in the <a href="#">SET_CONDITION</a> on page 165 command.</p> </div>
	<p>1ST ALLOYING ELEMENT: &lt;ELEMENT NAME&gt;</p> <p>The first alloying element must be given.</p> <p>All alloying elements are asked for in a sequence. These can be given in any order. You must know if you are present as assessed systems in the database. There is no error or warning messages if data are missing. Check the documentation of the database selected.</p> <p>If an alloy is selected, a list of legal alloying elements and their maximum percent is listed on-line.</p>
	<p>MASS (WEIGHT) PERCENT: &lt;AMOUNT OF THE ABOVE SPECIFIED ELEMENT&gt;</p> <p>The amount of the alloying element in mass (weight) percent. Using the DEFINE_MATERIAL command you cannot use the normal flexibility of Thermo-Calc for conditions, but all must be given in mass percent. However, you can afterwards change the conditions using the SET_CONDITION command.</p>
	<p>2ND ALLOYING ELEMENT: &lt;ELEMENT NAME&gt;</p> <p>The second alloying element must be given. If only one, press &lt;Enter&gt;. If an element name is given then the program asks for its mass fraction.</p>
	<p>MASS (WEIGHT) PERCENT: &lt;AMOUNT OF THE ABOVE SPECIFIED ELEMENT&gt;</p> <p>The amount of the above specified alloying element in mass (weight) percent.</p>
	<p>NEXT ALLOYING ELEMENT: &lt;ELEMENT NAME&gt;</p> <p>Continue giving elements and mass (weight) fractions until all elements specified. When all alloying elements and their compositions (as in the above prompt) are specified, press &lt;Enter&gt; as answer to this question to finish the materials definition.</p>
	<p>TEMPERATURE (C) /1000/: &lt;TEMPERATURE OF INTEREST IN OC&gt;</p>



Syntax	DEFINE_MATERIAL
	<p>POLY makes the first calculation after retrieving the data for this temperature. By pressing &lt;Enter&gt; to accept the default temperature. The value should be given in Celsius (oC).</p> <p> The pressure is set to 1 bar.</p>
	<p>REJECT PHASE(S) /NONE/: &lt;LIST OF PHASE(S) TO BE REJECTED&gt;</p> <p>This is a question generated by the database allowing you to select the phases. Normally, all phases should be included when you press &lt;Enter&gt;. If a phase is to be rejected, the name of the phase must be supplied. Several phase names can be specified in one line. It is possible to reject all phase by giving an asterisk *. If the number of phases to be included is much smaller than the total number of phases, it may be convenient to first reject all phases and then restore those that should be included. The question is repeated until you press &lt;Enter&gt; after rejecting all unwanted phases or an asterisk *.</p>
	<p>RESTORE PHASE(S) /NONE/: &lt;LIST OF PHASE(S) TO BE RESTORED&gt;</p> <p>You can restore phases that are accidentally or deliberately rejected. It may also be possible to restore some hidden phases.</p> <p>If phases are to be restored the name of the phases must be supplied. Several phase names can be specified in one line. It is possible to restore all phase by giving an asterisk *. The question is repeated until you press &lt;Enter&gt; after restoring all desired phases.</p>
	<p>OK? /Y/: &lt;Y OR N&gt;</p> <p>All phases to be selected from the database are listed and the selection confirmed. If there are any errors or you want to amend the selection, answer N and you are returned to the question about rejecting phase(s).</p> <p>If the selection is confirmed by answering Y the software retrieves all thermodynamic data and available references from the chosen database.</p>
	<p>SHOULD ANY PHASE HAVE A MISCIBILITY GAP CHECK? /N/: &lt;Y OR N&gt;</p> <p>The database usually creates two or more composition sets for phases that can have miscibility gaps. However, for some phases this is not done automatically, for example the miscibility gap in the bcc phase in Fe-Cr is usually ignored. But if it is important to include a Cr-rich bcc phase, specify this here. It costs some computation time and may make the subsequent MAP or STEP more difficult to converge.</p> <p>If you do not want to have any phase with a miscibility gap in the calculation, press &lt;Enter&gt;. Then, the DEFINE_MATERIAL command starts calculating the equilibrium, and is terminated.</p>
	<p>To set such a phase with miscibility gaps in the calculation, answer Y. Then the software</p>

Syntax	DEFINE_MATERIAL
	<p>asks questions about the phase names and their constitutions, such as:</p> <pre>PHASE WITH MISCIBILITY GAP: &lt;PHASE NAME&gt;</pre> <p>You must supply the phase name, which has a miscibility gap under the specified system and conditions.</p>
	<pre>MAJOR CONSTITUENT(S) FOR SUBLATTICE #: /AA/: &lt;CONSTITUENT(S)&gt;</pre> <p>The software shows a default constituent in the sublattice # (1, 2, 3, ...), according to the existing phase definition in the chosen database. You can specify one or more major constituents for the sublattice # in the phase.</p> <p>This question is repeated until all sublattices are specified.</p>
	<pre>PHASE WITH MISCIBILITY GAP: &lt;PHASE NAME&gt;</pre> <p>You can supply another phase name with a miscibility gap under the specified system and conditions, and answer the questions concerning the major constituent(s) in associated sublattice(s).</p> <p>By pressing &lt;Enter&gt;, the command starts calculating the equilibrium, and then terminates.</p>
	<p> It is also possible to use this command to select an alloy from a specific database (e.g. the TCNI Ni-based Superalloys Database). Such alloys are predefined by the OPTION keyword inside the database, and have their default major elements and composition limits of their alloy elements.</p> <p>Such alloys available in the selected database (at the prompt <code>Database /ABCDE/</code> can be listed on the screen if typing a ? mark on the prompt <code>Major element or alloy</code>. When a specific predefined alloy (instead of a major element) is selected, the major element is staked from the alloy definition and shown on the screen (with a message like <code>Alloy found with major element NI</code>).</p> <p>You can only specify alloying elements and the compositions (weight percent or mole percent). Typing a ? at any of the prompts for the alloying element names, e.g. <code>1st alloying element</code>, <code>2nd alloying element</code>, lists all the alloying elements and the composition limits in the alloy. If the composition of an alloying element is outside of its limit, there is a message (such as <code>Amount above limit: 30.0000</code>) and a prompt <code>Override limit ? /N/</code>. If you decide to enforce the override by answering <code>Y</code> on this prompt (i.e. accepting the over-limit alloying composition), another warning message (such as <code>Amount of major element below limit: 70.0000</code>) and prompt <code>Override limit ? /N/</code>. Then further decide if enforcing the overriding: if <code>Y</code> then accepting the major element's composition below the limit; if <code>N</code> then using the predefined</p>

Syntax	DEFINE_MATERIAL
	major element composition limit.

## DELETE\_INITIAL\_EQUILIBRIUM

Delete ONE specific initial equilibrium point or ALL of the initial equilibria. The initial equilibria are used as starting points for all the sub-sequential MAP and STEP calculations.



Also see [ADD\\_INITIAL\\_EQUILIBRIUM](#) on page 119.

Syntax	DELETE_INITIAL_EQUILIBRIUM
Prompt	NUMBER /ALL/: <NUMBER OF AN INITIAL EQUILIBRIUM>
	Specify the number of an initial equilibrium (as a specific digit e.g. 3, or ALL) to be deleted from the POLY3 workspaces. It is recommended to use <a href="#">LIST_INITIAL_EQUILIBRIA</a> on page 157 to figure out the numbers for all the existing initial equilibrium points that have already been added ( <i>manually</i> through <a href="#">ADD_INITIAL_EQUILIBRIUM</a> on page 119, or <i>automatically</i> by some other POLY commands) and stored in the current POLY3 workspace. By default, ALL the initial equilibrium points are deleted.

## DELETE\_SYMBOL

Delete symbols (i.e. constants, variables, functions or tables. These symbols are entered with [ENTER\\_SYMBOL](#) on page 72.

Syntax	DELETE_SYMBOL
Prompt	NAME: <NAME OF A SYMBOL> Specify the name of the symbol to be deleted. Only one symbol can be deleted each time.

## ENTER\_SYMBOL

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

Functions or tables (with defined functions as values) can be entered in the POST module after a stepping or mapping calculation, for purposes of plotting such entered functions or tables as axis variables.

Within the POLY module, symbols are normally defined prior to an equilibrium calculation (enforced by a C\_E command), stepping calculation (enforced by the command [STEP\\_WITH\\_OPTIONS](#) on page 172) or mapping calculation (enforced by [MAP](#) on page 158). These can be entered after an equilibrium calculation; however, for defined functions, variable or tables, it requires using [EVALUATE\\_FUNCTIONS](#) on page 155 before showing the corresponding values in the calculated equilibrium state.


The symbols entered in the POST module are not saved in the currently-loaded POLY3 workspaces. Therefore, if you want to apply such symbols in other similar calculations for the same defined system, you must use the ENTER\_SYMBOL command prior to the STEPPING or MAPPING calculation in the POLY module.




Also see [ENTER\\_SYMBOL](#) on [page 72](#) for the GIBBS Module.



See example 44 in the *Console Mode Examples Guide* for an example of using variables and functions.


Syntax	ENTER_SYMBOL
Prompt	<p>CONSTANT, VARIABLE, FUNCTION OR TABLE? /FUNCTION/: &lt;KEYWORD&gt;</p> <p>The Keyword can be specified as CONSTANT, VARIABLE, FUNCTION or TABLE.</p> <ul style="list-style-type: none"> <li>• <b>CONSTANTS</b> can only be entered once and is a means of using a name for a numeric value. For example, the value of 1 atmosphere in Pascal can be denoted by P0 after the command ENTER CONSTANT P0=101325. Defined constants can be used as values in condition assignments, for example, SET-COND P=P0.</li> <li>• <b>FUNCTIONS</b> are expressions of state variables or other functions. These expressions are saved, and whenever a function value is requested all functions are evaluated. The reason for this is that they may depend on each other.</li> <li>• <b>VARIABLES</b> are similar to functions because they can also be expressions of state variables. However, contrary to functions, they are only evaluated when they are entered or if they are explicitly named in an <a href="#">EVALUATE_FUNCTIONS on page 155</a> command. It is possible to enter a variable with a new expression any time. This expression is evaluated directly and its value stored as the value of the variable. Defined variables can be used as values in the SET-CONDITION command.</li> <li>• <b>TABLES</b> are used for listing results from the STEP or MAP commands. A table consists of a list of any number of state variables, functions or variables. Defined tables can also be used in the post-processor POST.</li> </ul> <p> There is a special connection between tables and variables. If a variable is used in a table, it is evaluated for each line of the table in the TABULATE command or when the table is used in a plot.</p>
	<p>NAME: &lt;NAME OF THE SYMBOL&gt;</p> <p>Each symbol has a unique name that must start with a letter and can have maximum 8 characters.</p> <p>Legal characters include letters (either UPPER or lower case), digits and underscore _. Any other special character, such as parentheses ( and ), plus +, minus -, slash / or \, full stop (.), are illegal for symbol names.</p> <p>You can enter the symbol name and the value or function on the same line, these must be separated with an equal sign =, for example, TC=T-273.15 or T_C=T273.15 which stands for a definition of temperature in Celsius. Otherwise, these questions are asked.</p>

Syntax	ENTER_SYMBOL
	 For different types of symbol (constant, function, variable or table), the questions have different prompts.
	<p>FUNCTION: &lt;DEFINITION FOR A FUNCTION OR VARIABLE&gt;</p> <p><i>Functions</i> and <i>variables</i> are evaluated from an expression of state variables or other functions, constants or variables. The expression is a FORTRAN-like expression and operators +, -, *, = and ** can be used (** only with integer powers).</p> <p>Unary functions like LOG, LOG10, EXP, SIN, COS and ERF can also be used. An expression can be continued on more than one line. An expression should be terminated by a semicolon (;) or an empty line (by pressing &lt;Enter&gt; at the next prompt).</p> <p>Examples of function expressions:</p> <ul style="list-style-type: none"> <li>• GM(LIQUID) : The Gibbs energy of liquid per mole component</li> <li>• H.T/4.184: The heat capacity of the system in calories</li> <li>• ACR(CR) /X(FCC, CR) : The activity coefficient for Cr in FCC</li> <li>• T-273.15: The temperature in Celsius</li> </ul> <p>&amp;: &lt;CONTINUATION OF THE DEFINITION FOR THE SYMBOL&gt;</p> <p>The ampersand &amp; means that you can continue to write the function on the new line if one line is not enough for the function. If you finish the function press &lt;Enter&gt; again.</p>
	<p>VALUE: &lt;VALUE FOR A CONSTANT&gt;</p> <p>A <i>constant</i> can only be assigned a numeric value once.</p>
	<p>VALUE OR EXPRESSION: &lt;VALUE OF EXPRESSION FOR A VARIABLE&gt;</p> <p>A <i>variable</i> can be assigned a numeric value or an expression. An expression is evaluated immediately and discarded. Only the numeric value is kept. This gives a possibility to save a value between calculations with different conditions because all state variables and functions are evaluated for the new conditions.</p>
	<p>VARIABLE(S) : &lt;VARIABLE(S) IN A TABLE&gt;</p> <p>A <i>table</i> consists of a list of state variables or functions. One way to obtain results from a STEP command is through a table.</p> <p>Example:</p> <pre>ENTER TABLE K=T,X(LIQ,C),X(LIQ,CR),ACR(C)</pre> <p>Which means that the table called K contains four columns, i.e. the temperature, the mole</p>

Syntax	ENTER_SYMBOL
	<p>fractions of C and Cr in the LIQUID phase, and the activity of C.</p> <p>To show the temperature in Celsius in a table, give the command ENTER FUNCTION <math>TC=T-273</math>; and then use the symbol TC in the table.</p> <p>&amp; &lt;CONTINUATION OF THE DEFINITION FOR THE TABLE&gt;</p> <p>The ampersand &amp; means that you can continue to write the table on the new line if one line is not enough for the table. If you finish the table press &lt;Enter&gt; again.</p>

## EVALUATE\_FUNCTIONS

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

Syntax	EVALUATE_FUNCTIONS
Prompt	<p>NAME(S) : &lt;NAME(S) OF DEFINED FUNCTION(S)&gt;</p> <p>The names of one or more entered functions or variables must be specified. By typing a wildcard *, all functions and variables are evaluated.</p> <p> Variables are evaluated only if these are explicitly named.</p>

## LIST\_AXIS\_VARIABLE

Syntax	LIST_AXIS_VARIABLE
	Lists all the axis variables for a stepping or mapping calculation that have already been set by <a href="#">SET_AXIS_VARIABLE on page 164</a> .

## LIST\_CONDITIONS

All the conditions that are set by the command SET\_CONDITION and the command-sequence CHANGE\_STATUS PHASE =FIXED <0 or 1 or alike>, are listed. The current conditions are also listed by the command LIST\_EQUILIBRIUM. The degree of freedom in the defined system is also shown up. If this is zero, you can perform a COMPUTE\_EQUILIBRIUM command. If it is larger than zero, some more conditions are required, and you must further set additional ones, using [SET\\_CONDITION on page 165](#) or [CHANGE\\_STATUS on page 135](#). If it is negative, a user has defined too many conditions and needs to take away the unnecessary ones, using the SET\_CONDITION command (with a value of NONE for the to-be-deleted condition) or CHANGE\_STATUS command (i.e. changing a FIXED status of a phase to another type of phase status, ENTERED or DORMANT or SUSPENDED).


Syntax	LIST_CONDITIONS
Example	<pre>P=100000, T=800, N(NI)=1E-1, N=1 FIXED PHASES FCC_A1=1 LIQUID=0    DEGREE OF FREEDOM 0</pre>

## LIST\_EQUILIBRIUM

The result (always in SI units) from the last calculated equilibrium is listed on screen or in a textual file.



You can also execute this command if no calculation is made or if the calculation fails. It is your responsibility to interpret the results accordingly.

Syntax	LIST_EQUILIBRIUM
Prompt	<p>OUTPUT TO SCREEN OR FILE /SCREEN/: &lt;FILE NAME&gt;</p> <p>The name of the text file where the list of the calculation results shall be written.</p>
	<p>OPTIONS /VWCS/: &lt;OPTION(S)&gt;</p> <p>Select the output units and formats by optionally specifying a combination of these letters.</p> <ul style="list-style-type: none"> <li>• <i>Fraction order:</i> V means VALUE ORDER; A means ALPHABETICAL ORDER.</li> <li>• <i>Fraction type:</i> W means MASS FRACTION; X means MOLE FRACTION.</li> <li>• <i>Composition:</i> C means only COMPOSITION; N means CONSTITUTION and COMPOSITION.</li> <li>• <i>Phase:</i> S means including only STABLE PHASES; P means including ALL NON-SUSPENDED PHASES.</li> </ul>
	<p>Default options are VWCS. If the output fraction type should be in mole fraction (rather than mass fraction), then give VXCS or type X (implying that in this case the options V, C and S are accepted as the listing manners for fraction order, composition and phase).</p> <p>If accepting all the default options, or if accepting all the altered options that had already changed when using this command previously, you can type <code>L_E, , ,</code> or <code>LIST_EQUILIBRIUM , , ,</code></p> <p> LIST_EQUILIBRIUM displays ORD (ordered) or DISORD (disordered) (when available). See <a href="#">CHANGE_LEGEND</a> on page 193 for details.</p>




## LIST\_INITIAL\_EQUILIBRIA

List all the equilibria added with [ADD\\_INITIAL\\_EQUILIBRIUM](#) on page 119.

Syntax	LIST_INITIAL EQUILIBRIA
	All the initial equilibria are used for the MAP (and STEP) calculations.

## LIST\_STATUS

In the POLY module, list the status of components, species or phases.

Syntax	LIST_STATUS
Prompt	<p>Specify what to list:</p> <p>OPTION /CPS/: &lt;KEYWORD(S)&gt; KEYWORD = C OR P OR S, OR ANY COMBINATION</p> <ul style="list-style-type: none"> <li>• C means list component status</li> <li>• P means list phase status</li> <li>• S means list species status</li> <li>• CS for both components and species</li> </ul> <p>Default is CPS.</p>
	<p>The results depend on the key word specified in the options for <a href="#">CHANGE_STATUS</a> on page 59, a table with the current status of phases or species or components, or the combinations, is shown:</p> <ul style="list-style-type: none"> <li>• For components, the statuses and reference states are listed.</li> <li>• For species, only the status is listed.</li> <li>• For ENTERED and FIXED phases, the status, driving forces and equilibrium amounts are listed.</li> </ul>
	<p> The metastable phases are listed in descending order of stability. To avoid long outputs only 10 metastable phases (in ENTERED status) are listed by lines, while all other less stable phases are merged onto one line. For DORMANT phases, their phase names and driving forces are listed. For SUSPENDED phases, only the phase names are listed.</p>

## LIST\_SYMBOLS

For both the POLY and POST modules, list the definitions for all constants, functions, variables and tables.

In order to find the value of a function or variable, use [SHOW\\_VALUE](#) on page 172 or [EVALUATE\\_FUNCTIONS](#) on page 155. A table is tabulated with the TABULATE command.

Syntax	LIST_SYMBOLS
	The defined variables are listed up together with the defined functions, but variable names are followed by a percentage sign %.


## LOAD\_INITIAL\_EQUILIBRIUM

Copies all conditions and calculated results from a specific added initial equilibrium to the current equilibrium. The current conditions and calculation results are lost, and the newly loaded initial equilibrium point gets into the POLY workspace.

Syntax	LOAD_INITIAL_EQUILIBRIUM
Prompt	<p>NUMBER: &lt;NUMBER OF AN INITIAL EQUILIBRIUM&gt;</p> <p>Specify the number of an initial equilibrium to be loaded as current. The number can be found with <a href="#">LIST_INITIAL_EQUILIBRIA</a> on the previous page.</p>

## MAP

This command starts the mapping procedure for making a calculation of phase diagrams in a defined multicomponent heterogeneous system, from one or more initial equilibria. A phase diagram is usually mapped within a specific space that is constructed by two (or more) defined independent mapping axis-variables.

Syntax	MAP
	<div>  <p>A phase diagram consists of mapped phase boundary lines/curves; on one side of each such phase-boundary line/curve, the amount of one specific stable phase is zero (i.e. the zero-fraction lines). From a single MAP calculation, many different types of phase diagrams in the defined multicomponent heterogeneous system can be plotted, with some desired properties (that vary along the calculated phase-region boundaries) plotted as X/Y-axis variables. All different types of phase diagrams are generated by the mapping calculations through this command.</p> </div>

Normally, you need to have calculated at least one initial equilibrium point and have also defined at least two independent varying variables (i.e. the controlling conditions in the system) that are set with [SET\\_AXIS\\_VARIABLE](#) on page 164. You can also have three, or four or maximum five independent varying variables that are defined by the SET\_AXIS\_VARIABLE command).

This lists the current values of each of the independent axis variables for each of the calculated equilibrium points along each of the mapped phase boundaries, and also lists the corresponding information when the set of stable phases changes.

The Global Minimization Technique is by default enforced in this command while it can be disabled if having decisively switched it off (or possibly in some special modules) through changing the minimization option using the [ADVANCED\\_OPTIONS](#) on page 125 → MINIMIZATION\_OPTION command-sequence. You can choose how often to do a Global Minimization test (via the Global Test Interval option) in the ADVANCED\_OPTIONS STEP\_AND\_MAP command-sequence.

During a MAP calculation, the values of mapped axis-variables for presenting each phase boundary (lines/points) of the calculated phase-regions are listed, and the corresponding stable-phase sets are shown up. You can terminate the mapping of a line by pressing a single CTRL-A (Windows) or CTRL-C (Linux). This can be useful in order to stop a longish calculation without losing what is already calculated.

If there is any convergence problem in finding a stable solution at a certain stage during a calculation procedure enforced by this command, these messages display on screen:

```
Convergence problems, increasing smallest site-fraction from 1.00E-30 to hardware
precision 2.00E-14. You can restore using SET-NUMERICAL-LIMITS
```

This implies that smallest site fraction in the current POLY3 workspace is automatically increased from the default value 1.00E-30 to the hardware-dependent precision (under Linux, as 2.00E-14). For other subsequent POLY-module calculation in the current TC run, you can use the POLY command [SET\\_NUMERICAL\\_LIMITS](#) on page 168 to restore or reset the smallest site fraction to the previous or another preferred value, as well as to reset other numerical limits.

In particular, for phase diagrams with tie-lines in the plane (i.e. most binary systems and ternary isotherms), there is a MAP procedure which checks for the best phase to use as axis variables in order to ensure reasonable increments between the tie-lines. This produces smoother curves and also gives a better stability in finding adjacent phase-regions.

Complex miscibility gaps of various solution phases are automatically detected during a mapping calculation, and two or more composition sets for each of such solution phases are automatically generated as well, through an automatic Global Minimization Test procedure (by specifying a Global Test Interval value and confirming the Automatically add initial equilibria in the ADVANCED\_OPTION STEP\_AND\_MAP command-sequence). As a particular case, such an automatic Global Minimization Test ensures that you can start calculating from high temperatures in an austenitic steel (metallic FCC\_A1 solution phase) where the MC carbides/nitrides/carbonitrides (i.e. the C-/N-rich sides of the FCC\_A1 miscibility-gap, often (while not always) being referred to as FCC\_A1#2, FCC\_A1#3, etc.) are not stable, and during the MAP command the MC carbides/nitrides/carbonitrides may first become metastable with a composition different from the metallic FCC\_A1 phase and later also stable. The advanced mapping procedure (enforced by the Global Minimization Technique) inside the Thermo-Calc

software (both the Console Mode and Graphical Mode) can efficiently and effectively handle complex miscibility gaps in multicomponent heterogeneous systems.

To get a complete phase diagram, sometimes it may be necessary to have multiple starting equilibrium-points, and/or to have added multiple initial-equilibrium points (through [ADD\\_INITIAL\\_EQUILIBRIUM](#) on page 119) inside various phase-region boundaries under certain direction(s).

## POST

Syntax	POST
	Switches to the post-processor (the POST module), which has its own command repertoire.
	 See <a href="#">POST Commands</a> on page 188 for all details.

## READ\_WORKSPACES

The POLY3 and GIBBS workspaces and the calculated results from the MAP and STEP commands can be READ from a file where they are saved with [SAVE\\_WORKSPACES](#) on page 30. Such an \*.POLY3 file is not printable.

Syntax	READ_WORKSPACES
Options	<p><code>File name</code> is the name of a saved POLY3-file where the POLY3 and GIBBS workspaces shall be read from must be specified. You do not need to type the extension if it is the default *.POLY3 (Windows) or *.poly3 (Linux), otherwise type the whole POLY-file name.</p> <p>A window opens so that the path (in the <b>Look in</b> field) and <b>File name</b> can be specified. The <b>Files of type</b> (i.e. POLY3) cannot be changed. Click <b>Open</b> to open the POLY3 and GIBBS workspaces from the saved *.POLY3 file.</p>
	<p>When reading back an original POLY3 workspace that has already been saved as an *.POLY3 file in the current Thermo-Calc (Console Mode) run or had been read from an existing POLY3 file under the current work area, while some additional changes in the settings may be made but do not need to be kept in further steps in the current Thermo-Calc (Console Mode) run or any diagram is plotted in the POST module, you can type <code>READ, ,</code> or <code>READ_WORKSPACE , ,</code></p>

## RECOVER\_START\_VALUES

Syntax	RECOVER_START_VALUES
	Recovers the start values in equilibrium calculations.

## REINITIATE\_MODULE

Ensures that the whole POLY module (and thus the entire POLY workspace) is reinitiated to the state as it was when first entered.

Syntax	REINITIATE_MODULE
	All the defined components, defined conditions, changed status, entered symbols, defined independent axis-variables, calculated starting equilibrium-points, added initial equilibrium points, stepped/mapped equilibrium data, and so forth, are removed completely. The saved file name is restored to the default.

## SAVE\_WORKSPACES

Thermo-Calc allows saving the current status and workspaces of the program, including thermodynamic data, conditions, options and results from a single, stepping or mapping calculation on an \*.POLY3 file. Do this for later use or when you need to terminate the current Thermo-Calc (Console Mode) run.

The POLY3 and GIBBS workspaces are saved on a file with this command. In the GIBBS workspace, all thermochemical data are stored. In the POLY3 workspace, all thermochemical data, all the last set of conditions and equilibrium state, changed status, entered symbols, advanced options, defined stepping/mapping variables, added initial equilibria, stepped/mapped results, etc., are stored, so it also contain the GIBBS workspace. After a SAVE\_WORKSPACE command, you can always come back to exactly the state you had when you issued the SAVE\_WORKSPACE command by giving a READ\_WORKSPACE command.

After saving the POLY3 and GIBBS workspaces on a file, you can leave the program and at a later time READ the file and continue from the saved state.




A STEP or MAP command automatically saves the work file with the most lately specified name. Do not SAVE after a MAP or STEP.

The results from the STEP or MAP commands are destroyed by the SAVE\_WORKSPACE command. You may append several results obtained by sequential STEP or MAP calculations without destroying the previous results, whilst SAVE\_WORKSPACE erases them all. Keeping this in mind is important and useful particularly for calculating various isothermal (or isoplethal) sections and plotting them on the same diagram in a single Thermo-Calc run.

You may append several results by STEP or MAP without destroying the previous results but the SAVE command erases them all. To suspend some of the STEP or MAP results, use the AMEND\_STORED\_EQUILIBRIA command.

When you go to a response-driven module such as POTENTIAL or SCHEIL for example, a workspace file is automatically opened. In the workspace file, system definitions, conditions for the calculation, calculation results, and plot settings is saved. The file is saved in the current working directory, and is named after the name of the module that created it. For example, the POTENTIAL module saves a

workspace file called POT.POLY3 (or POT.poly3 in Linux); the POURBAIX module saves a file called POURBAIX.POLY3; etc.

Syntax	SAVE_WORKSPACES
Options	<p>A <code>file name</code> must be specified. The default extension of the POLY workspace file is <code>*.POLY3</code> (Windows) or <code>*.poly3</code> (Linux), while you can have any other extension.</p> <p>A <b>Save</b> window displays, so that the path (in the <b>Save in</b> field) and <b>File</b> name can be specified. The file type (i.e. POLY3) in the <b>Files of type</b> cannot be changed.</p>
	<p> When saving a POLY3 workspace under a name that already exists under the current work area, which is saved by default (after running a special module, e.g. BIN, TERN, POT, SCHEIL and POURBAIX) or in an earlier stage of the current Thermo-Calc (Console Mode) run or in a previous run (which is READ into the current POLY3 workspace), you can type <code>SAVE,,y</code> or <code>SAVE_WORKSPACE , , y</code>. However, this must also be avoided if some results from previous MAP or STEP calculations shall not be destroyed.</p>

## SELECT\_EQUILIBRIUM


If you create more than one initial equilibrium (during data-assessments using the PARROT/ED\_EXP modules), you can switch between them using this command.

Syntax	SELECT_EQUILIBRIUM
Prompt	<p>NUMBER /NEXT/: &lt;CHOICE ON EQUILIBRIUM&gt;</p> <p>Answer FIRST, LAST, NEXT, PREVIOUS or PRESENT.</p>
	<p>Most commands affect only the PRESENT equilibrium. However, the commands <a href="#">REINITIATE_MODULE</a> on the previous page and <a href="#">DEFINE_COMPONENTS</a> on page 143 remove all the stored equilibria.</p>

## SET\_ALL\_START\_VALUES

Set start values, e.g. if the calculation fails or if you have a miscibility gap or ordering. If temperature and pressure are not conditions, you are asked for values of them. Then for each phase prompt on if it should be stable and on its constitution.

Syntax	SET_ALL_START_VALUES
	<p>T /XXXX/: &lt;TEMPERATURE IN K&gt;</p> <p>If the temperature is not a condition, supply a guess of its final value (in K).</p>
	<p>P /100000/: &lt;PRESSURE IN PA&gt;</p>

Syntax	SET_ALL_START_VALUES
	If the pressure is not a condition supply a guess of its final value (in pa).
Prompts	<p>AUTOMATIC START VALUES FOR PHASE CONSTITUTIONS? /N/: &lt;Y, N OR F&gt;</p> <p>Answer N (the default), Y or F (for force).</p> <p>The reason for the F option is that in some cases the calculation has failed because impossible conditions are set, e.g. <math>W(C) = 1.5</math> [<math>W(C)</math> is mass fraction and must thus be less than unity]. The program tries to fulfil this condition by putting maximum amount of carbon in all phases, but can fail anyway. When you detect the error and set <math>W(C)</math> to 0.015, the calculation may still fail because it could start from the previous values. To get back to 'fresh' start values, give the answer F for FORCE.</p> <p>If Y this command immediately terminates, and the program automatically sets the start values for phase constitutions in all possible phases.</p> <p>For N supply an initial amount of each entered phase and the major constituents or site fraction of each constituent.</p>
	<p>SHOULD &lt;PHASE&gt; BE STABLE /N/: &lt;Y/1 OR N/2&gt;</p> <p>A guess on if this phase should be stable or not is requested. All entered phases are prompted for this question and next two.</p> <div style="border: 1px solid black; padding: 10px; margin: 10px 0;">  <p>You cannot have more phases stable than you have components, but at least one (which dissolves all constituents) must be set as stable. For backward compatibility, this question can be answered by 1 (for Yes) or 0 (for No).</p> </div> <p>The phase name may have a hash sign # followed by a digit, e.g. BCC_A2#2. For phases with miscibility gaps, there should be two phases with the same name but with different numbers after the hash sign.</p>
	<p>MAJOR CONSTITUENT(S) : &lt;NAME OF MAJOR CONSTITUENT(S) IN THE PHASE&gt;</p> <p>The constituent with the largest fraction in the phase should be specified. If there are more than one constituent with a large fraction, give them all on the same line. If the default major constituents should be used answer with an asterisk (*). By giving \$ the constitution is not changed. If there should be no major constituent give NONE and or if the major constituent(s) are improperly specified, you are asked for individual fractions in the phase.</p>
	<p>Y (&lt;PHASE&gt;, &lt;CONSTITUENT&gt;) /.XXXXXXXXX/: &lt;.YYYYY&gt;</p> <p>The current value (.XXXXXXXXXX) is default. You can accept the default by pressing</p>

Syntax	SET_ALL_START_VALUES
	<p>&lt;Enter&gt; or give a new value (.YYYYY).</p> <p>The phase name or constituent name may have a hash sign # followed by a digit, e.g. Y (BCC_A2#2, FE) , Y (BCC_A2#2, C#2) . For phases with miscibility gaps, there should be two phases with the same name but with different numbers after the hash sign. For phases with sublattices, the constituents in sublattice 2 or higher is also be suffixed with a hash sign # followed by a digit.</p>

## SET\_AXIS\_VARIABLE

In order to calculate a diagram, set at least one axis variable in a stepping calculation, or at least two axis variables in a mapping calculation. For property diagrams, one axis is enough; for phase diagrams two or more are necessary. Any condition that can be set to calculate an equilibrium can be used as an axis variable (with its lower and upper limits and step length) by using the SET\_AXIS\_VARIABLE command, and the POLY program does, after a STEP or MAP command, vary the value of the condition between the limits set on its related axis variable. As an extraordinarily unique and powerful feature of the Thermo-Calc software, up to five independent axis variables can possibly be used in a mapping calculation of a multicomponent heterogeneous system; however, the axis numbers 3, 4 and 5 must have chemical potentials of components (or temperature or pressure) as conditions.

Syntax	SET_AXIS_VARIABLE
	<p>AXIS NUMBER /#/: &lt;AN AXIS NUMBER&gt;</p> <p>Specify a number between 1 and 5. The axis numbers 3, 4 and 5 must have chemical potentials of components (or temperature or pressure) as conditions.</p>
Prompts	<p>CONDITION /NONE/: &lt;ONE CONDITION&gt;</p> <p>Here the condition that should be varied along the axis must be given. The condition is specified as in <a href="#">SET_CONDITION on the next page</a>, for example W (C) for mass fraction of carbon. By accepting NONE, the axis is removed.</p>
	<p>MIN VALUE /0/: &lt;MIN VALUE&gt;</p> <p>Specify the minimum value of the axis condition.</p>
	<p>MAX VALUE /1/: &lt;MAX VALUE&gt;</p> <p>Specify the maximum value of the axis condition.</p>
	<p>INCREMENT /.025/: &lt;STEP LENGTH&gt;</p> <p>Specify the maximum step length. By default, this is 1/40 of the total axis length.</p>

You can give the SET\_AXIS\_VARIABLE command without having set a condition on the axis variable. Under such circumstances, the relevant condition is automatically created and the value set between the



minimum and maximum axis limits; however, as a side effect, the POLY module creates two conditions,  $P=1e5$  and  $N=1$  (these have not been defined as a condition yet), in case you set an axis variable which is not already a condition.

You can use a logarithmic axis during calculations. This is useful for low fractions like in a gas phase where  $1e-7$  to  $1e-2$  might be an interesting range. The pressure is also suitable for logarithmic step. You specify the logarithmic axis by giving an asterisk  $*$  after the increment value.



The increment in this case is treated as a factor.

For example,

```
S-A-V 1 P 1E5 1E25 5*
```

This makes axis 1 a logarithmic axis where the difference between two calculated values makes a factor 5.




The factor must be larger than 1.0.

In some cases, such as when the `DEFINE_DIAGRAM` command is used or a special advanced module (e.g. `BIN`, `TERN`, `POT`, `SCHEIL` or `POURBAIX`) is called, some axis variables are automatically set by the program, not necessarily by this command.

## SET\_CONDITION

Specify the equilibrium conditions for the calculation. All kinds of state variables, as well as most of the M/W/V/F-suffixed state variables (for normalization) and R-suffixed state variables (with respect to chosen reference states), can be used as conditions. Beside temperature and pressure conditions, a multicomponent system can have mixed types of conditions; this brings the extreme flexibility and powerfulness to the complex calculations with the Thermo-Calc software system. You should repeat this command for a multicomponent system, till the degree of freedom in the defined system becomes zero. When a `FIXED` phase status is used on a specific phase (use [CHANGE\\_STATUS](#) on page 135), it is equivalent to one condition (implying that particular phase is stable in the defined system).

Syntax	<b>SET_CONDITION</b>
	<p>Each condition must be given explicitly, but can be given on the same line (separated by a comma (,) or an empty space) or on separate lines with each one started with the command.</p> <p><b>Example</b></p> <pre>SET_COND T=1273, P=1E5, W(C)=.0015, X(LIQ,Cr)=.22, ACR(N)=.2</pre> <p>or</p> <pre>SET_COND T=1273, P=1E5 SET_COND W(C)=.0015, X(LIQ,Cr)=.22 ACR(N)=.2</pre> <p>In this example, the temperature is set to 1273 K, the pressure to 1 bar (1E5 Pascal), the mass (weight) fraction of C to 0.0015 and the mole fraction of Cr to 0.22 and the activity of N to 0.2.</p>
Prompt	<p>STATE VARIABLE EXPRESSION: &lt;STATE VARIABLE NAME OR LINEAR EXPRESSION&gt; OR A LINEAR EXPRESSION OF STATE VARIABLES.</p> <p>Some of the state variables that can be used in conditions are:</p> <ul style="list-style-type: none"> <li>• T: temperature in the system (in K)</li> <li>• P: pressure in the system (in Pascal)</li> <li>• N: system size (mole number in moles)</li> <li>• B: system size (mass in grams)</li> <li>• N(&lt;component&gt;) : mole number of a component in the system</li> <li>• X(&lt;component&gt;) : mole fraction of a component in the system</li> <li>• W(&lt;component&gt;) : mass fraction of a component in the system</li> <li>• ACR(&lt;component&gt;) : activity of a component in the system</li> <li>• MUR(&lt;component&gt;) : chemical potential of a component in the system</li> <li>• X(&lt;phase&gt;,&lt;component&gt;) : mole fraction of a component in a phase</li> <li>• W(&lt;phase&gt;,&lt;component&gt;) : mass fraction of a component in a phase</li> <li>• ACR(&lt;species&gt;,&lt;phase&gt;) : activity of a species in a solution phase</li> <li>• MUR(&lt;species&gt;,&lt;phase&gt;) : chemical potential of a species in a solution phase</li> <li>• H: enthalpy in the system (in J)</li> <li>• HM(&lt;phase&gt;) : enthalpy of a phase (in J/mol)</li> </ul>

Syntax	SET_CONDITION
	<p>There are many state variables that can be used in conditions. For more information, enter an <code>INFO STATE_VARIABLES</code> command. A condition is normally a value of a single state variable with its value.</p> <p><b>Example</b></p> <pre>T=1273.15  P=1E5 X(C)=.002 W(CR)=0.5 ACR(CR)=0.85 X(FCC,C)=.001 H=-250000 HM(BCC)=-225000</pre> <p>A condition can also be a value of a linear expression involving more than one state variable. For example,</p> <pre>X(LIQ,S)-X(PYRR,S)=0</pre> <p>This means that it is a condition that the mole fraction of <code>S</code> component should be the same in the LIQUID and PYRRHOTITE phases. In practice, that should be the congruent melting point.</p> <p> After the equal sign only a numeric value is allowed in the expression.</p>
	<p>FACTOR: &lt;A FACTOR FOR THE STATE VARIABLE, OR A CONTINUATION&gt;</p> <p>This question means you did not answer the previous question. The program is then expecting a single state variable or a complete state variable expression, or the numeric factor in an expression with only one state variable. In a state variable expression a state variable may be preceded by a constant factor. An example of this is:</p> <pre>2*MUR(Fe)+3*MUR(O)=-35000</pre> <p>This means that it should be a condition that two times the chemical potential of <code>Fe</code> plus three times the chemical potential of <code>O</code> should be -35000 J/mol.</p>
	<p>STATE VARIABLE: &lt;A SPECIFIED STATE VARIABLE, OR A CONTINUATION&gt;</p> <p>This question is prompted if a single state variable name has not given in either the prompt <code>State variable expression</code> or <code>Factor</code>, or a state variable expression is given but the expression is incomplete, for example, <code>T-</code> or <code>2*MUR(Fe)+</code>, for which the program is then expecting a continuation of the unfinished expression. You need to specify a state variable or a complete state variable expression, or complete the unfinished state variable</p>

Syntax	SET_CONDITION
	expression. If a numeric factor is given before this prompt, only one state variable can be specified; otherwise, the program only takes the first state variable to complete the expression (i.e. the factor times the state variable).
	<p>VALUE /X/: &lt;A NUMERIC VALUE, A CONSTANT OR A VARIABLE&gt;</p> <p>The value of the condition. This can be a numeric value, a constant or a variable. A suggestion is given as the default value. The special value <code>NONE</code> means that the condition is removed; for example <code>T=NONE</code> takes away the temperature condition.</p>


## SET\_INPUT\_AMOUNTS

Specify how a system is made up from mixing of various substances. It is useful with a substance database. In the C-H-O-N system, you can, for example, give:

```
S-I-A N(H2)=10, N(H2O)=25, N(C1O2)=5, N(N2)=100
```

The POLY module automatically converts this into conditions for the current set of components. In the case when the elements are defined as the components, the command above is equivalent to

```
SET-CONDITION N(H)=70, N(O)=35, N(C)=5, N(N)=200
```

Syntax	SET_INPUT_AMOUNTS
Prompts	<p>QUANTITY: &lt;N(&lt;SPECIE&gt;) OR B(&lt;SPECIE&gt;)&gt;</p> <p>You can give the amount also preceded with an equal sign = [e.g. <code>N(H2)=10</code> or <code>B(H2O)=1000</code>], or press &lt;Enter&gt; for the next prompt on the amount of the quantity.</p>
	<p>AMOUNT: &lt;VALUE OF THE QUANTITY&gt;</p> <p>Specify the numerical value of the quantity.</p> <p> You can give negative amounts in the SET-INPUT-AMOUNTS command.</p>

## SET\_NUMERICAL\_LIMITS

Change the criteria for convergence. This is to speed up a calculation in a complex system.

If there is any convergence problem in finding a stable solution at any stage during a calculation procedure enforced by [COMPUTE\\_EQUILIBRIUM](#) on page 139, [STEP\\_WITH\\_OPTIONS](#) on page 172, [MAP](#) on page 158 or [ADVANCED\\_OPTIONS](#) on page 125), this message displays:

```
Convergence problems, increasing smallest site-fraction from 1.00E-30 to hardware
precision 2.00E-14. You can restore using SET-NUMERICAL-LIMITS
```

This implies that smallest site fraction in the current POLY3 workspace is automatically increased from the default value 1.00E-30 to the hardware-dependent precision (under Linux, as 2.00E-14). For other

subsequent POLY-module calculation in the current Thermo-Calc (Console Mode) run, you can use this command to restore or reset the smallest site fraction to the previous or another preferred value, as well as to reset other numerical limits.

Syntax	SET_NUMERICAL_LIMITS
Prompt	<p>MAXIMUM NUMBER OF ITERATIONS /200/: &lt;XXX&gt;</p> <p>By default, the program tries 500 iterations before it gives up. As some models give computation times of more than 1 CPU second/iteration, this number is also used to check the CPU time and the calculation stops if 500 CPU seconds/iterations are used.</p>
	<p>REQUIRED ACCURACY /1E-6/: &lt;YYY&gt;</p> <p>This is a relative accuracy, and the program requires that the relative difference in each variable must be lower than this value before it has converged. A larger value normally means fewer iterations but less accurate solutions. The value should be at least one order of magnitude larger than the machine precision.</p>
	<p>SMALLEST FRACTION /1E-12/: &lt;ZZZ&gt;</p> <p>This is the value assigned to constituents that are unstable. It is normally only in the gas phase you can find such low fractions.</p> <p>The default value for the smallest site-fractions is <math>1\text{E}-12</math> for all phases, except for IDEAL phase with one sublattice site (such as the GAS mixture phase in many databases) for which the default value is always as <math>1\text{E}-30</math> (unless you have used the SET_NUMERICAL_LIMITS command to reset an even-lower value (e.g. <math>1\text{E}-45</math>, that is naturally enforced to all the phases in the system).</p>
	<p>APPROXIMATE DRIVING FORCE CALCULATION FOR METASTABLE PHASES /Y/: &lt;Y OR N&gt;</p> <p>Normally the POLY module only requires that the set of stable phases is in equilibrium in order to terminate the iterations. The metastable phases are included in all iterations but these may not have reached their most favourable composition and thus their driving forces may be only approximate [corresponding to Y]. You can also force the calculation to converge for the metastable phases by answering N if it is important that these driving forces are correct, which may require more iterations, and the STEP and MAP command may also terminate due to bad convergence in a metastable phase.</p>


## SET\_REFERENCE\_STATE

The reference state for a component is important when calculating activities, chemical potentials and enthalpies. The reference state for a component is determined by the database. For each component the data must be referred to a selected phase, temperature and pressure, i.e. the reference state. All data in all phases where this component dissolves must use the same reference state. However, different databases may use different reference states for the same element. Thus you must be careful when, for example, mixing data from different databases.

By default, activities, chemical potentials, etc. are computed relative to the reference state used by the database and this may thus differ depending on the database. With this command select the reference state for a component if the reference state in the database does not suit.

You can set the reference state for a component as `SER`, i.e. the Stable Element Reference (which is usually set as default for a major component in alloys that is dominated by the component). Under such a case, the temperature and pressure for the reference state is not needed and thus is not prompted.

In order to specify conditions in the specified reference state, you can append an `R` to the state variables. Thus, `AC` is the activity (of a system component or of a species in a phase) with respect to the default reference state, and `ACR` is the activity with respect to the selected reference state; `MU` is the chemical potential of a system component with respect to the default reference state, and `MUR` stands for the chemical potential with respect to the selected reference state. The `AC` and `ACR` variables, for both components in a system and species in a phase, can be specified in natural logarithm, e.g. `LNAC(Fe)`, `LNACR(C)`, `LNAC(O2,GAS)`, `LNACR(O2,GAS)`.

Syntax	SET_REFERENCE_STATE
Prompts	<p>COMPONENT: &lt;NAME OF THE COMPONENT&gt;</p> <p>The name of the component must be given.</p>
	<p>REFERENCE PHASE: &lt;NAME OF A PHASE USED AS THE NEW REFERENCE STATE&gt;</p> <p>The Name of a phase, that must be either ENTERED or DORMANT or SUSPENDED, must be given here. The component must, of course, be a constituent of this phase.</p> <p>For a phase to be usable as reference for a component the component need to have the same composition as an end member of the phase. The reference state is an end member of a phase. For example, in the Fe-C system, BCC can be a reference state for Fe but not for C since BCC cannot exist as pure C.</p> <p>If a component has the same composition as several end members of the chosen reference phase, then the end member is selected that at the specified temperature and pressure has the lowest Gibbs energy. For example, setting the reference state for component O as gas (one sublattice) with constituents O1, O2 and O3 results in O2 being the reference state if, at the present temperature, pure O2 has the lowest energy of O1, O2 and O3. If the reference state is set above a critical higher temperature, then O1 has the lowest energy and consequently become the reference state.</p> <p> The actual calculation of the reference state is only performed when SET_REFERENCE_STATE is executed. For example, if GAS is chosen as the reference phase of component O at such a high temperature that O1 has the lowest energy, then O1 remains the reference state even at calculations performed at lower temperatures where O2 has a lower energy than O1.</p>
	TEMPERATURE /*/: <TEMPERATURE FOR THE REFERENCE STATE>

Syntax	SET_REFERENCE_STATE
	Select the temperature (in K) for the reference state. The wildcard value * means the current temperature is used for the calculation.
	<p>PRESSURE /1E5/: &lt;PRESSURE FOR THE REFERENCE STATE&gt;</p> <p>Select the pressure (in Pa) for the reference state. The wildcard value * means the current pressure is used for the calculation.</p>
	<p><b>Examples</b></p> <pre>S-R-S Fe SER S-R-S Cr FCC * 100000 S-R-S H2O AQUEOUS * 100000 S-R-S ZE REF_ELECTRODE * 100000</pre>

## SET\_START\_CONSTITUTION

This command is similar to [SET\\_ALL\\_START\\_VALUES](#) on page 162, but is used for an individual phase that may have a wrong constitution.

Syntax	SET_START_CONSTITUTION
	<p>PHASE NAME: &lt;NAME OF A PHASE, AND POSSIBLE MAJOR CONSTITUENT(S)&gt;</p> <p>Specify the name of a phase for which the constitution shall be set.</p>
Prompts	<p>If there is a major constituent of the phase, you must specify this on the same line as the phase name. By giving an *, select the default major constituents. A \$ means keeping the same constitution, and NONE means to give individual site-fractions.</p>
	<p>Y(&lt;PHASE&gt;#&lt;COMPOSITION_SET&gt;,&lt;CONSTITUENT&gt;#&lt;SUBLATTICE&gt;) /XXX/: &lt;SF&gt;</p> <p>The site fraction (SF) of the constituent shall be given. The default value xxx is the last calculated one.</p>

## SET\_START\_VALUE

Set a start value of an individual variable.





This command is not often required as the automatic start values can be handled for most problems.

Syntax	SET_START_VALUE
Prompts	STATE VARIABLE: <NAME OF A STATE VARIABLE> The state variable must be given.
	VALUE Specify the value to be assigned the state variable as start value.

## SHOW\_VALUE

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

Syntax	SHOW_VALUE
Prompt	STATE VARIABLE OR SYMBOL: <NAME(S) OF STATE VARIABLE(S) OR SYMBOL(S)> A single or several state variables or symbols (entered functions or variables) can be specified.
	<p> The wildcard * can be used to denote all phases or all components.</p> <p>You can use the dollar-sign \$ to denote all stable phases. Thus, the command SHOW W (*,*) lists the mass fraction of all phases, whereas SHOW W (\$, *) lists the mass fraction of all stable phases.</p> <p> If you SHOW a function, all functions are evaluated using the current values of the state variables. But if you SHOW a variable, it retains its value from the time it was ENTERED or last EVALUATED.</p> <p>Therefore to save a value from one calculation to another, ENTER it to a variable. This is frequently done in the PARROT module to transfer values between equilibria.</p>

## STEP\_WITH\_OPTIONS

Initiates the stepping procedure to make a calculation of property diagrams in a multicomponent heterogeneous system. A property diagram is usually stepped under one defined independent stepping axis-variable, and is often constructed by the defined independent mapping axis-variable against a chosen property (for the system, or for a specific phase, or for a certain species).





A property diagram consists of property lines that change (normally) along with the stepping axis-variable. From a single STEP calculation, many different types of property diagrams in the defined multicomponent heterogeneous systems can be plotted. Various types of property diagrams are generated by the stepping calculations through this STEP\_WITH\_OPTION command

Normally, before it can be invoked, you must have already calculated an initial equilibrium point and have also set one independent varying variable (i.e. the controlling condition in the system) using [SET\\_AXIS\\_VARIABLE](#) on page 164.

The Thermo-Calc Console Mode lists the current values of the axis variable for each calculated equilibrium, as well as the corresponding information when the set of stable phases changes.

The Global Minimization Technique is by default enforced in this command (STEP), while it can be disabled if having decisively switched it off by a user (or possibly in some special modules) through changing the minimization option using the [ADVANCED\\_OPTIONS](#) on page 125 → MINIMIZATION\_OPTION command-sequence.

You can choose how often to do a Global Minimization Test (via the `Global Test Interval` option) in the `ADVANCED_OPTIONS STEP_AND_MAP` command-sequence.

- **NORMAL:** Allows a stepping calculation with the chosen independently-varying equilibrium condition (axis-variable).
- **INITIAL\_EQUILIBRIA:** An initial equilibrium is stored at each calculated equilibria. It is intended to generate a matrix of calculated initial equilibria, first stepped under a STEP INITIAL\_EQUILIBRIA command-sequence and then repeated by another STEP NORMAL command-sequence (or even continued by a MAP command). For example, you can first use the temperature condition as the stepping axis-variable, and give a STEP INITIAL\_EQUILIBRIA command sequence; this calculates a number of initial equilibrium points and automatically ADDs each one as an initial equilibria for another STEP NORMAL command-sequence (or even for a MAP command). Before the second STEP command (i.e. the STEP NORMAL command-sequence), you can alternatively chose a compositional condition as the new stepping axis-variable; then the STEP NORMAL command-sequence uses those created starting equilibrium points (at different temperatures) and steps in such a new compositional variable. As a result, these two sequential STEP commands together give a matrix of values. Actually, you can carry this option even deeper.
- **SEPARATE\_PHASES:** Each of the entered phases are calculated separately and in parallel at each step, i.e. all the phases are calculated for the same composition (if the phases exist for that composition). In this way, you can calculate how the Gibbs energy for a number of phases varies for varying compositions; and this option is particularly useful for calculating Gibbs energies for complex phases with miscibility gaps and for ordered phase which is never disordered (e.g. SIMGMA-phase, G-phase, MU-phase or alike).


However, this option may sometimes be unable to find all the ordered phases and their disordered pairs during a STEP SEPARATE\_PHASES calculation; and it is thus recommended to always use the newer ONE\_PHASE\_AT\_TIME option instead, for STEPPING heterogeneous systems with both ordered phases and their disordered pairs.

- **ONE\_PHASE\_AT\_TIME**: The stepping calculation is conducted for only one phase at a time individually (stepped over the whole stepping variable range), but the stepping is repeated for all the entered phase in the defined system. This new option is particularly useful for properly stepping in composition for an equilibrium heterogeneous system with both ordered phases and their disordered pairs, because of that, instead of calculating for the same composition for each of the phases at each composition step, it at least starts the stepping in each of the phases in the default most-stable compositions (the major constitutions). Therefore, this option is always recommended for STEPPING heterogeneous systems with both ordered phases and the disordered pairs.
- **EVALUATE**: The variables given are evaluated after each step, which may change other conditions. This option is useful for performing the Ordinary ScheilGulliver Approach (non-equilibrium transformations) for simulating alloy solidifications without back diffusion of fast-diffusing interstitial components in solid phases. However, users are always recommended to go directly to the SCHEIL module and run the desired Scheil-Gulliver type of simulations in a much easy, straightforward and automatic way.
- **MIXED\_SCHEIL**: A stepping calculation designed for the Extended Scheil-Gulliver Approach (partial-equilibrium transformations) to simulate alloy solidifications with back-diffusion of one or more fast-diffusing interstitial components (such as C, N, O, S, etc.) in solid phases is performed. However, you are always recommended to go directly to the SCHEIL module and run the desired Scheil-Gulliver type of simulations in a much easy, straightforward and automatic way.
- **T-ZERO**: T<sub>0</sub> (T-zero) lines in a diffusionless transformation [where two specific partially-equilibrated phases have the same Gibbs energy] are calculated along a composition variable (set as the stepping variable).
- **PARAEQUILIBRIUM**: The paraequilibrium state in a partly partitionless transformation [under which two partially-equilibrated phases have the same chemical potential (but different contents) for one or more interstitial components, such as C, N, O, S, etc.] is calculated along varied temperature or along a composition variable (of the matrix or one substitutional component).


Syntax	step_with_options
Prompt	OPTION? /NORMAL/: <A CHOSEN OPTION, N OR I OR S OR O OR E OR M OR T OR P>
Options	<p><b>Choose from these options</b></p> <p>Allows a stepping calculation with the chosen independently-varying equilibrium condition (axis-variable). By repeating the STEP NORMAL command-sequence, you can make several stepping calculations while still keep all the stepping-calculation results in the same current POLY3 workspaces (saved in the same RESULT . POLY3 file default-named by the program, or in the same &lt;MyName&gt; . POLY3 file that is specified before the first STEP NORMAL command-sequence).</p> <p><input checked="" type="checkbox"/> Only when there is no SAVE_WORKSPACES command issued before the repeated STEP NORMAL command-sequence, such repeated stepped results can be restored into the same current POLY3 workspaces/file.</p> <p>Choose to alter one or more controlling conditions for calculating starting equilibrium point(s) and can also optionally change the independently-varying condition (stepping-variable) and its settings for the stepping. All such alternations/changes are properly stored into the current POLY3 workspaces/file.</p> <p>Therefore, with one or more repeated STEP NORMAL command-sequence (without any SAVE_WORKSPACES command in between for overwriting stepped results), it enables you to easily/efficiently generate some special types of property diagrams and even to plot special phase boundary lines on phase diagrams, as described below:</p> <p>Calculate/plot missing part(s) of a specific property [that are calculated under another controlling condition inside the range of the stepping-variable] on the same property diagram.</p> <p>Calculate/plot two or more sets of a specific property [that are calculated under different controlling conditions and stepped over the same stepping-variable range] on the same property diagram for the same system.</p> <p>Calculate some special phase-boundary lines [especially for some defined secondary phase transformations or alike, e.g. the BCC_A1 &lt;--&gt; BCC_B2 phase-boundary, or equal-Gm for two specific phases, or equal-fraction or equal-activity for a certain species in two specific phases, that shall be calculated under different controlling-conditions and also be stepped over different stepping variable(s)], and then plot (or impose) them onto a corresponding phase diagram (which can be resulted from several such STEP NORMAL calculations or even from a separate</p>


NORMAL

Syntax	step_with_options
	MAP calculation) for the same system.
INITIAL_ EQUILIBRIA	<p>An initial equilibrium stored at every step. This option has not been completely implemented yet. It is intended to make a stepping calculation by generating a matrix of calculated initial equilibria, first stepped under a STEP INITIAL_EQUILIBRIA command-sequence and then repeated by another STEP NORMAL command-sequence (or even continued by a MAP command). For example, you can first use the temperature condition as the stepping axis-variable, and give a STEP INITIAL_EQUILIBRIA command-sequence; this calculates a number of initial equilibrium points and automatically ADDs each one as an initial equilibria for another STEP NORMAL command-sequence (or even for a MAP command). Before the second STEP command (i.e. the STEP NORMAL command-sequence), you can chose a compositional condition as the new stepping axis-variable; then the STEP NORMAL command-sequence uses those created starting equilibrium points (at different temperatures) and steps in such a new compositional variable. As a result, these two sequential STEP commands together give a matrix of values.</p>
SEPARATE_PHASES	<p>Each phase is calculated separately. This option performs a stepping calculation in which all the entered phases in the system are calculated separately and in parallel at each step, i.e. all the phases are calculated for the same composition (if the phases exist for that composition). In this way, you can calculate how the Gibbs energy for a number of phases varies for varying compositions. This option is useful when you want to plot <math>G_m</math> curves versus composition for a given temperature, particularly for calculating the Gibbs energy differences for phases with miscibility gaps and for ordered phase which is never disordered (e.g. SIMGMA-phase, G-phase, MU-phase or alike). However, this option may sometimes be unable to find all the ordered phases and their disordered pairs during a STEP SEPARATE_PHASES calculation procedure; and it is thus recommended to always use the newer ONE_PHASE_AT_TIME option instead, for STEPPING heterogeneous systems with both ordered phases and their disordered pairs.</p>
ONE_PHASE_AT_ TIME	<p>One phase calculated at a time and repeated for all entered phase. It allows a stepping calculation for only one phase at a time individually (stepped over the whole stepping variable range), but the stepping is repeated for all the entered phase in the defined system.</p> <p>The STEP ONE_PHASE_AT_TIME command-sequence properly STEP in composition for an equilibrium heterogeneous system with both ordered phases and their disordered pairs, instead of calculating for the same composition for each of the phases at each composition step, and it at least starts the stepping in each of the phases in their default most-stable compositions (the major constitutions). Therefore, this option is always recommended for STEPPING</p>


Syntax	step_with_options
	heterogeneous systems with both ordered phases and their disordered pairs.
EVALUATE	<p>Specified variables evaluated after each step. This is an advanced option for experts of Thermo-Calc, when additional conditions (rather than the stepping variable) should be changed during a stepping calculation. It allows a stepping calculation in a single axis with simultaneous evaluation of one or more variables after each step. As variables can be used as conditions, it means that you can change the conditions during the stepping. After a successful STEP EVALUATE calculation, you can go to the POST module to manually define and plot various desired property diagrams.</p> <p>Specify the prompt:</p> <p>VARIABLE NAME(S) : &lt;VARIABLE NAME&gt;</p> <p>The names of the variables that shall be evaluated after each step must be typed here.</p> <p>During a STEP EVALUATE calculation in some earlier TCC versions, it used to calculate all kinds of property diagrams, phase fraction plots, etc., some problems may occur, especially when new phases want to appear. These problems are simplified by the general improvement of convergence but a number of additional fixes are added to the STEP EVALUATE command-sequence to handle the problems. The miscibility gap test is automatically used during stepping (see the command <a href="#">ADVANCED_OPTIONS</a> on page 125) if a phase has two or more composition sets.</p> <p>The miscibility gap test means that you can now start calculating from high temperatures in a steel, where the MC carbide is not stable; and during a STEP EVALUATE calculation procedure, the MC carbide first becomes metastable with a composition different from the metallic FCC phase and later also stable.</p> <p>One good case of using this advanced option is described in the command <a href="#">INFORMATION</a> on page 5 with the subject as SOLIDIFICATION (Solidification Path Calculations). With this option, you can simulate the Ordinary Scheil-Gulliver Solidification Processes (i.e. non-equilibrium transformations) by changing the overall composition to the new liquid composition after each step, but without considering back-diffusion of fast-diffusing interstitial components in solid phases.</p> <p> See example 30A in the <i>Console Mode Examples Guide</i>. It is recommended to go directly to the SCHEIL module and run the desired Scheil-Gulliver type of simulations.</p>


Syntax	step_with_options
MIXED_SCHEIL	<p>Extended Scheil-Gulliver type solidification with back diffusion.</p> <p>This option leads to a stepping calculation (always with T as the stepping axis variable) for simulating Extended Scheil-Gulliver solidification processes (i.e. <i>partial-equilibrium transformations</i>) with considering back-diffusion of one or more fast-diffusing interstitial components (such as C, N, O, S, etc.) in formed solid phases; it also allows considering BCC→FCC phase transformation (practically for steels) along the alloy solidification process.</p> <p>To ensure a successful stepping calculation of mixed Scheil-Gulliver simulation of solidification process of a defined alloy system with a certain initial overall composition, it is important to pay special attention to the following four aspects, before performing this advanced-option stepping calculation:</p> <p>For solution phases with possibility of miscibility gap existence, you have appropriately added the necessary composition set(s);</p> <p>You have already set the temperature condition as the stepping</p> <p>SET_AXIS_VARIABLE command, with a minimum and maximum temperature points as well as an appropriate s temperature step for the cooling process); It is equally important there must be a composition condition for each of the back-diffusion components (i.e. fast-diffusing interstitial components, such as C, N and/or other elements) that are already defined in terms of mole-fraction or mass-fraction, e.g. <math>X(C)</math> and <math>W(N)</math>. Otherwise, a stepping calculation with this option can fail.</p> <p>An initial equilibrium in which the LIQUID mixture phase is the only stable must be calculated [for this reason, it is always good to start with a relatively high temperature condition for the initial equilibrium calculation; and it is always necessary to reject or suspend the GAS mixture phase (if exists) before the C-E and STEP commands, to avoid its formation along with LIQUID].</p> <p>In cases where fast-diffusing interstitial components are specified as back-diffusion components, there is a possibility to choose an option to allow BCC&gt;FCC phase transformation (practically for steels) during the alloy solidification process.</p> <p>With this stepping calculation option, these prompts need to be specified:</p> <p>FAST DIFFUSING COMPONENTS: &lt;FAST DIFFUSION INTERSTITIAL(S)&gt;</p> <p>Specify one or more interstitial component(s) as the back-diffusion component(s).</p> <p>If there is only one fast-diffusing interstitial component (e.g. C or N), type its name at the prompt;</p>


Syntax	step_with_options
	<p>If there are two or more fast-diffusing interstitial components (e.g. C, N and S), always type their names on the same line at once (separated by an empty space in between, e.g. C N S);</p> <p>If there is no fast-diffusing interstitial component to be considered, type <code>NONE</code> to ignore back diffusion entirely, meaning a normal Scheil-Gulliver simulation is performed.</p> <p> Such specified back-diffusion interstitial component(s) must be appropriately defined according to the phase constitution definitions of some major alloy solution phases (e.g. FCC, BCC, HCP, etc.): These are located on the interstitial/vacancy sublattices in such alloy solution phases; otherwise, such a Scheil-Gulliver simulation may not make sense at all.</p> <p><code>ALLOW BCC -&gt; FCC ? /Y/: &lt;Y OR N&gt;</code></p> <p>Type <code>Y</code> (or press &lt;Enter&gt; to accept the default) or <code>N</code> to allow or not allow the <code>BCC-&gt;FCC</code> phase transformation (which is usually a typical phenomenon along the cooling processes of steels/Fe-alloys).</p> <p>During the <code>STEP MIXED_SCHEIL</code> calculation procedure, the simulated solidification path, including the locally-equilibrated phase assemblage (region), captured temperature condition (<code>T</code> in K), remaining liquid phase (<code>NL</code>, mole fraction), overall formed solid phases (<code>NS</code>, mole fraction) and latent heat formation (<code>NH</code>, J/mol) along the cooling process are shown after the information on starting temperature point of the alloy solidification process, e.g.</p> <pre> Solidification starts at 1743.15 K Phase Region from 1.744150E+03 for: LIQUID Phase Region from 1.742525E+03 for: LIQUID FCC_A1#1 1742.5250      0.9960      0.0040      -1.1824 1742.4000      0.9795      0.0205      -202.1585 . . . . . Phase Region from 1.733150E+03 for: LIQUID BCC_A2 FCC_A1#1 </pre>

Syntax	step_with_options			
	1733.1500	0.3294	0.6707	-8032.6240
	1733.0250	0.3237	0.6763	-8095.1490
	. . . . .			
	<p>After a successful STEP MIXED_SCHEIL calculation, you can go to the POST module to manually define and plot various property diagrams for the alloy solidification process according to the chosen Scheil-Gulliver model, or to impose existing relevant experimental information or other types of calculated solidification results [e.g. Scheil-Gulliver simulation with or without considering fast-diffusing interstitial component(s), full-equilibrium approach, or Diffusion Module (DICTRA)-type simulation with moving-boundary conditions] onto the same plotted property diagrams. Normally, the solidus temperature (<math>T</math> in Celsius) is set as one of the axis variables (usually as Y-axis in most cases), while the other plotted quantity on the other axis can be the amount of overall formed solid alloy phases (<math>NS</math> in mole-fraction or <math>BS</math> in mass-fraction), the amount of remaining liquid phase (<math>NL</math> in mole-fraction or <math>BL</math> in mass fraction), the heat of latent along the solidification process (<math>NH</math> in J/mol or <math>BH</math> in J/gram), among many other properties in the solidified alloy phases or in the whole alloy system.</p> <p>However, you are always recommended to go directly to the SCHEIL module and run the desired Scheil-Gulliver type of simulations in a much easy, straightforward and automatic way.</p>			
T-ZERO	<p>T0 lines between two specific phases calculated This option allows a stepping calculation of the so-called T0 (T-zero) line in a <i>diffusionless transformation</i> [where two specific partially-equilibrated phases have the same Gibbs energy, along a composition variable which has already set as the stepping variable with <a href="#">SET_AXIS_VARIABLE</a> on page 164.</p> <div style="border: 1px solid black; background-color: #d4edda; padding: 10px; margin: 10px 0;">  <p>The temperature condition cannot be set as the stepping variable if you want to make a STEP T-ZERO calculation.</p> </div> <p>To ensure a successful calculation of T0 line between two specific phases after an initial equilibrium calculation in the current system, it is recommended to make a single T0 point calculation by the ADVANCED_OPTION T-ZERO command-sequence, prior to performing this STEP T-ZERO command-sequence, although this might not be always necessary for some systems.</p> <p>Specify these prompts:</p> <p>NAME OF FIRST PHASE: &lt;PHASE A&gt;</p> <p>NAME OF SECOND PHASE: &lt;PHASE B&gt;</p>			




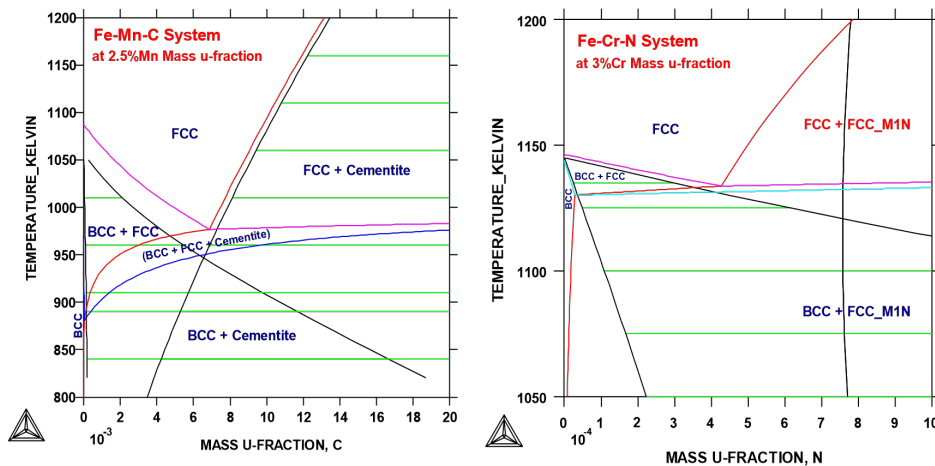
Syntax	step_with_options
	<p>The names of the two target phases, for which the Gibbs energies equal to each other at each point on the T0 line, must be typed at the above two prompts subsequently.</p> <p>During the STEP T-ZERO calculation procedure, the calculated T0 values are shown after the corresponding scanned conditions (of the stepping composition variable), e.g.</p> <pre> Phase Region from 1.000000E-01 for:     BCC_A2     FCC_A1 1.000000E-01      940.24 9.250000E-02      941.20 . . . . . 2.500000E-03      977.61 7.500000E-09      979.34 Phase Region from 1.000000E-01 for:     BCC_A2     FCC_A1 1.000000E-01      940.24 1.075000E-01      939.62 . . . . . 2.950000E-01      1084.87 3.000000E-01      1080.99 </pre> <p>After a successful STEP T-ZERO calculation, you can go to the POST module to plot the T0 line against the stepping composition variable or another varying axis, or to impose the calculated T0 line onto a normal phase diagram [normally plotted as a T-X isopleth].</p> <p> See examples 23 and 41 in the <i>Console Mode Examples Guide</i>.</p>
PARAEQUILIBRIUM	<p>Praequilibrium state between two specific phases is calculated with this. It allows a stepping calculation of so-called praequilibrium lines in a partly partitionless transformation between two specific partially-equilibrated phases in an alloy system where the chemical potential for one or more fast-diffusing interstitial components but not for the substitutional components in two specified phases are equal.</p>

Syntax	step_with_options
	<p>Therefore, the STEP PARAEQUILIBRIUM command-sequence ensures that the two partially equilibrated phases have the same chemical potential (but different contents) for one or more fast-diffusing interstitial components (such as C, N, O, S, etc., as individual or combined)), along varied temperature or along a composition variable (of the matrix or one substitutional component) which has already set as the stepping variable with <a href="#">SET_AXIS_VARIABLE</a> on page 164.</p> <p>More than one interstitial components can be treated as fast-diffusion species (such as C, N, O, S, etc., as individual or combined) in a paraequilibrium stepping calculation.</p> <p> The composition condition for the interstitial components cannot be set as the stepping variable if you want to make a STEP PARAEQUILIBRIUM calculation.</p> <p>To ensure a successful stepping calculation of paraequilibrium states between two specific phases in a defined alloy system, it is important to first make a starting-point equilibrium calculation with an initial overall composition in the current system before performing this advanced-option stepping calculation; however, it is unnecessary to obtain an equilibrium in which either one or both of the target phases is stable. The initial overall composition must have a reasonable setting for the desired paraequilibrium calculation for the two target phases. This is especially true for cases where there are more than one interstitial components to be considered in the paraequilibrium state, because different interstitial components (for example C and N combined) may have significant different behaviours as partitioning into different structured phases; otherwise, for one chosen interstitial component the initial overall composition is OK for the paraequilibrium calculation between the specified two phases, but for other chosen interstitial component(s) it might be impossible to calculate the paraequilibrium state.</p> <p>Always check if the chosen <code>phaseA</code> and <code>phaseB</code> have the exact same definition of elements and if the chosen interstitial components are all in the vacancy sublattice sites of the two phases; otherwise the program cannot find the paraequilibrium state (as it is impossible to correctly calculate u-fractions).</p> <p>Always have a comprehensive understanding of the normal phase diagram for the currently investigated system, so that you make the appropriate choice of the phase pair and starting bulk composition for the system.</p> <p>Always set the status of the chosen interstitial components as SPECIAL using the command:</p>

Syntax	step_with_options
	<pre>CHANGE_STATUS COMPONENT &lt;interstitial component&gt; = SPECIAL</pre> <p>By doing this, you get a clear picture on u-fractions of various substitutional and interstitial components, which are different from the overall composition in the system. The SPECIAL status means that specified component(s) are not included in summations for mole or mass fractions. Therefore, all the composition variables plotted from the paraequilibrium calculations are u-fraction related quantities.</p> <p>Always make a single-point paraequilibrium calculation by the command-sequence of ADVANCED_OPTIONS PARAEQUILIBRIUM, prior to performing this STEP PARAEQUILIBRIUM command-sequence, although this might not be always necessary for some systems.</p> <p>With this stepping calculation option, these prompts need to be specified:</p> <pre>NAME OF FIRST PHASE: &lt;PHASE A&gt; NAME OF SECOND PHASE: &lt;PHASE B&gt;</pre> <p>The names of the two target phases A and B, between which the paraequilibrium states establish, must be typed at the above two prompts subsequently or on the same (first) line at once (separated by an empty space, e.g. FCC BCC, FCC#2 M23C6).</p> <div style="border: 1px solid black; background-color: #d4edda; padding: 10px; margin: 10px 0;">  <p>It is important to understand that this is the calculation of a paraequilibrium state between the two specified phases.</p> </div> <p>Particularly, there are four issues which you need to consider:</p> <ol style="list-style-type: none"> <li>1. Both chosen phases must have similar interstitial/vacancy sub-lattices where the fast-diffusion interstitial component(s) occupy.</li> <li>2. The choice on the target phase pair must be reasonable for the defined system and specified initial overall composition.</li> <li>3. Both target phases should have phase constitution definitions that cover all the defined substitutional and interstitial components of the current alloy system; or</li> <li>4. It is impossible to calculate the paraequilibrium state between the target phase pairs with given interstitial component(s) in the currently defined system.</li> </ol>

Syntax	step_with_options
	<p>FAST DIFFUSING COMPONENT: /C/: &lt;INTERSTITIAL COMPONENT(S)&gt;  FAST DIFFUSING COMPONENT: /NONE/: &lt;INTERSTITIAL COMPONENT(S)&gt;</p> <p>The name(s) of the fast-diffusing interstitial component(s) (C as the default single component) must be given either one by one at each of the above prompts subsequently or in a combination (separated by an empty space in between, e.g. C N S) at the same (first) prompt; otherwise, press &lt;Enter&gt; key to start the paraequilibrium line stepping-calculation.</p> <p>Note the following:</p> <p>Such specified fast-diffusing interstitial component(s) must be appropriately defined according to the phase constitution definitions of the two selected phases: These must be located on the interstitial/vacancy sublattices in both chosen phases.</p> <p>If there is only one fast-diffusing component which is carbon, press &lt;Enter&gt; to accept the default value (C) at the first prompt; if the single fast-diffusing interstitial component is another element (e.g. N), appropriately type interstitial component the name at the first prompt;</p> <p>If there are two or more fast-diffusing components (e.g. C and N), type their names at the above prompts subsequently or at the same (first) prompt (separated by an empty space, such as C N);</p> <p>To finish the input of fast-diffusing elements, accept NONE at a repeated prompt;</p> <p>If NONE or a non-existing component name is typed at the first prompt, it means no back diffusion is to be considered, and the para-equilibrium calculation is thus cancelled entirely.</p> <p>During the STEP PARAEQUILIBRIUM calculation procedure, the calculated paraequilibrium states include the:</p> <ul style="list-style-type: none"> <li>• corresponding stepping conditions (e.g. temperature in K, or the stepping composition variable of the matrix component or of one of substitutional components) which has already set as the stepping variable by the SET_AXIS_VAR command);</li> <li>• amounts of the phase A in mole number [i.e. NP (phaseA) ];</li> <li>• amounts of the phase B in mole number [i.e. NP (phaseB) ];</li> <li>• contents of the interstitial component(s) in the phase A expressed in u-fractions [i.e. u-f (phaseA, component (s) ) ];</li> </ul>

Syntax	step_with_options
	<ul style="list-style-type: none"> <li>contents of the interstitial component(s) in the phase B expressed in u-fractions [i.e. <math>u-f(\text{phaseB}, \text{component}(s))</math>];</li> <li>LNACR(component) value(s) for the interstitial(s).</li> </ul> <p>After a successful STEP PARAEQUILIBRIUM calculation, you can go to the POST module to plot a paraequilibrium phase diagram, or to impose the calculated paraequilibrium states onto a normal phase diagram [normally plotted as a T-X isopleth with one of the considered interstitial component(s) as the x-axis variable].</p> <p> See examples 23 and 42 in the <i>Console Mode Examples Guide</i>.</p> <p>However, the stepping calculation procedure for the currently specified paraequilibrium states between the two specified phases may find difficulties at some steps due to some possible numerical problems (normally regarding to the u-fractions of the interstitial components under some composition ranges), or it may completely fails. In the latter case, it implies that the chosen target phase pair may be unreasonable for the defined alloy system or for the defined initial overall composition, or one or both phases may have inappropriate phase constitution definitions regarding the specified interstitial component(s) and substitutional components. Then, you must either modify the settings of initial overall composition or specify the reasonable target phase pair with an appropriate choice of the fast diffusion interstitials in the defined alloy system.</p>



The figure above shows the plot of a paraequilibrium calculation of isopleths: Formation of para-pearlite in two Fe-based alloys, with equilibrium results appended.

- ✓ The calculated paraequilibrium phase boundaries (black lines) are shown with tie-lines (in green-colour). In the Fe-2.5Mn-C alloy system, C is considered as fast diffusing interstitial component in the BCC+FCC and FCC+Cementite paraequilibrium stepping calculations; while in the Fe-3Cr-N alloy system, N is treated as fast diffusing interstitial components in the BCC+FCC and FCC+FCC\_M1N (i.e. FCC#1+FCC#2) paraequilibrium stepping calculations.
- ✓ During a STEP calculation, the value of the stepping axis variable for each calculated equilibrium is listed and also the set of stable phases.

You can stop the mapping of a line by pressing a single CTRL-A (under MS Windows) or CTRL-C (under Linux). This can be useful in order to stop a longish calculation without losing what is already calculated.

If there is any convergence problem in finding a stable solution at any stage during a calculation procedure enforced by a STEP\_WITH\_OPTIONS command-sequence, this message displays:

```
Convergence problems, increasing smallest site-fraction from 1.00E-30 to hardware
precision 2.00E-14. You can restore using SET-NUMERICAL-LIMITS
```

This implies that smallest site fraction in the current POLY3 workspace is automatically increased from the default value  $1.00\text{E-}30$  to the hardware-dependent precision (under Linux, as  $2.00\text{E-}14$ ). For other subsequent POLY-module calculation in the current TC run, you can use the POLY command [SET\\_NUMERICAL\\_LIMITS](#) on page 168 to restore or reset the smallest site fraction to the previous or another preferred value, as well as to reset other numerical limits.

Complex miscibility gaps of various solution phases are automatically detected during a stepping calculation, and two or more composition sets for each of such solution phases are automatically generated as well, through an automatic Global Minimization Test procedure (by specifying a `Global Test Interval` value and confirming the `Automatically add initial equilibria` in the `ADVANCED_OPTION STEP_AND_MAP` command-sequence). As a particular case, such an automatic Global Minimization Test ensures that you can now start calculating from high temperatures in an austenitic steel (metallic FCC\_A1 solution phase) where the MC carbides/nitrides/carbonitrides (i.e. the C-/N-rich sides of the FCC\_A1 miscibility-gap, often (while not always) being referred to as FCC\_A1#2, FCC\_A1#3, etc.) are not stable, and during the MAP command the MC carbides/nitrides/carbonitrides may first become metastable with a composition different from the metallic FCC\_A1 phase and later also stable.

Occasionally, it may be necessary to have a specified increment other than the default value for the defined stepping axis-variable, in order to calculate/plot a smoother property diagram.

To get a complete property diagram, sometimes (especially in some earlier Thermo-Calc versions) it may also be required to have more than one starting equilibrium-points (under another starting equilibrium condition), and repeat the stepping calculation over the same stepping axis-variable range (while without over-writing the same POLY3 workspaces via a `SAVE_WORKSPACE` command). However, using the current STEP procedure such a requirement become less necessary.

## TABULATE

For any entered table, this command gives a table of values from equilibria calculated with a STEP command. It works only for a table that is entered in either the POLY or POST module.



Unlike the TAB module's command (also called [TABULATE on page 253](#)) it is not possible to plot columns from the tabulated tables. For this use normal POST commands.

Syntax	TABULATE
Prompts	NAME: <NAME OF A TABLE ENTERED IN EITHER POLY OR POST> Specify a table name that is entered in either the POLY or POST module.
	OUTPUT ON SCREEN OR FILE /SCREEN/: <FILE NAME OR RETURN> Specify a file name if you want to save on a file the table values along the defined STEP calculation, or press <Enter> if want to see the table values displayed.

## POST Commands

The POST module (post-processor) is available from the POLY module. See [POLY\\_3 Commands](#) on page 117 for other information about the POLY module. Read [Using the POST Module](#) on page 190 before beginning.

In this section:

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<i>Using the POST Module</i> .....	190
<i>ADD_LABEL_TEXT</i> .....	190
<i>APPEND_EXPERIMENTAL_DATA</i> .....	192
<i>CHANGE_LEGEND</i> .....	193
<i>DUMP_DIAGRAM</i> .....	194
<i>ENTER_SYMBOL</i> .....	195
<i>FIND_LINE</i> .....	198
<i>LIST_DATA_TABLE</i> .....	198
<i>LIST_PLOT_SETTINGS</i> .....	199
<i>LIST_SYMBOLS</i> .....	199
<i>MAKE_EXPERIMENTAL_DATAFILE</i> .....	199
<i>MODIFY_LABEL_TEXT</i> .....	200
<i>PLOT_DIAGRAM</i> .....	200
<i>PRINT_DIAGRAM</i> .....	201
<i>QUICK_EXPERIMENTAL_PLOT</i> .....	201
<i>REINITIATE_PLOT_SETTINGS</i> .....	202
<i>RESTORE_PHASE_IN_PLOT</i> .....	202
<i>SELECT_PLOT</i> .....	202
<i>SET_AXIS_LENGTH</i> .....	203
<i>SET_AXIS_PLOT_STATUS</i> .....	203
<i>SET_AXIS_TEXT_STATUS</i> .....	203
<i>SET_AXIS_TYPE</i> .....	204
<i>SET_COLOR</i> .....	204

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<i>SET_CORNER_TEXT</i> .....	205
<i>SET_DIAGRAM_AXIS</i> .....	206
<i>SET_DIAGRAM_TYPE</i> .....	208
<i>SET_FONT</i> .....	209
<i>SET_INTERACTIVE_MODE</i> .....	209
<i>SET_LABEL_CURVE_OPTION</i> .....	209
<i>SET_PLOT_FORMAT</i> .....	210
<i>SET_PLOT_OPTIONS</i> .....	211
<i>SET_PLOT_SIZE</i> .....	212
<i>SET_PREFIX_SCALING</i> .....	213
<i>SET_RASTER_STATUS</i> .....	213
<i>SET_REFERENCE_STATE</i> .....	213
<i>SET_SCALING_STATUS</i> .....	214
<i>SET_TIC_TYPE</i> .....	215
<i>SET_TIELINE_STATUS</i> .....	215
<i>SET_TITLE</i> .....	215
<i>SET_TRUE_MANUAL_SCALING</i> .....	216
<i>SUSPEND_PHASE_IN_PLOT</i> .....	216
<i>TABULATE</i> .....	216

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## Using the POST Module

Use the POST module after a [STEP\\_WITH\\_OPTIONS](#) on page 172 or [MAP](#) on page 158 calculation to generate *graphical* or *tabulated* presentations on screen or into files.

The graphical files are available in different formats (e.g. PS, EMF, PNG, BMP, PDF, JPG, TIF) or data forms (e.g. EXP, TAB and WRL). The graphical output can be phase diagrams, property diagrams, diffusion profiles and other types of plots. The tabulated presentation is into a basic text file (TXT) or a spreadsheet (e.g. an MS Excel file with an extension of .XLS).

The POST module is available through these modules:

- POLY
- TAB
- BIN
- TERN
- POT
- SCHEIL
- POURBAIX

Within the POST module, you can choose any state variable, any derived variable, or any entered symbol (functions or variable) as the X/Y-axis.



Also see [Thermodynamic Variables and Units](#) on page 269.

When a diagram is plotted, appearance parameters for defining a high-standard graph can be further specified, e.g. curve labelling options, diagram titles and subtitles, plot size, axis length, axis types, axis-tic type, tie-line status, automatic or manual scaling and zooming, semi-automatic or manual labelling on phase boundaries and phase regions, graphic formats, text fonts, colours, raster plot, etc.

You can append experimental data onto a plotted diagram. You can also save the coordinates onto a textual file, which can be edited and used as an experimental data file to be merged onto another diagram or as a part of a setup file for PARROT-module assessment.

Phases can be suspended or restored in a plotted diagram. The reference states for components can also be modified for the resulted diagrams. Moreover, you can translate a plotted property diagram (after a stepping calculation) into a tabulated form, such as a simple list on screen or a textual file, and a spreadsheet .

## ADD\_LABEL\_TEXT

Add a text to an area in a phase diagram or a property diagram. The label is written starting from the specified coordinates. Optionally, you can also let the program automatically add the text by first

calculating an equilibrium state at the specified coordinates and then making a label out of the stable phase names.


The label texts and coordinates, either added by this command or modified with [MODIFY\\_LABEL\\_TEXT](#) on page 200 (or manually edited in the **Console Results** window), are stored in the workspace, and these may later be saved onto an \*.EXP file (with [MAKE\\_EXPERIMENTAL\\_DATAFILE](#) on page 199).







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



[Adding and Editing Plot Labels](#) on page 92 in the *Thermo-Calc User Guide*.

Syntax	ADD_LABEL_TEXT
Prompts	<p>GIVE X COORDINATE IN AXIS UNITS: &lt;VALUE OF THE X COORDINATE&gt;</p> <p>Specify the value of the X coordinate where the label is to start.</p>
	<p>GIVE Y COORDINATE IN AXIS UNITS: &lt;VALUE OF THE X COORDINATE&gt;</p> <div style="border: 1px solid black; background-color: #d4edda; padding: 10px; margin: 10px 0;">  <p>The labels disappear if any axis is changed afterwards.</p> </div> <p>Specify the value of the Y coordinate where the label is to start.</p>
	<p>AUTOMATIC PHASE LABELS? /Y/: &lt;Y OR N&gt;</p> <p>If you answer Y, the program automatically calculates the equilibrium at the given coordinates and generates a label with the names of the stable phases. However, the automatic calculation works only for phase diagrams that are mapped with two axes in the POLY module, and sometimes it may not work correctly especially for complex heterogeneous interaction systems; in such cases, a message displays.</p>
	<p>TEXT: &lt;TEXT FOR THE LABEL&gt;</p> <p>If you answer N enter text at the prompt. You can enter simple text, use LaTeX, rotate the text, as well as adjust the font size.</p> <p><b>LaTeX:</b> You can use LaTeX commands to enter text and symbols. First enter the command followed by the expression or string, for example to display Al<sub>2</sub>O<sub>3</sub> as subscripts:</p> <pre>\latex Mole-fraction Al_2O_3</pre>

Syntax	ADD_LABEL_TEXT
	<p> For a list of supported LaTeX commands, see <a href="http://www2.ph.ed.ac.uk/snuggletex/documentation/math-mode.html">http://www2.ph.ed.ac.uk/snuggletex/documentation/math-mode.html</a> .</p> <div style="border: 1px solid black; padding: 10px; margin: 10px 0;"> <p> By default when using the LaTeX command, you are in math mode and Thermo-Calc automatically interprets the entered text as math. The above link uses the dollar sign (\$) in all the examples but this is NOT required. For example, if you enter <math>E=mc^2</math> this is displayed including the \$ instead of the equation.</p> </div> <p> To add a mixture of plain text and equation text, you can exit math mode using the string <code>\textrm</code> followed by the text to display enclosed in curly brackets. For example <code>\latex \textrm{Mole-fraction }Al_2O_3</code> displays this label <code>Mole-fraction Al<sub>2</sub>O<sub>3</sub></code> .</p> <p><b>Rotate the text:</b> If you want to rotate the label, start a text string with the rotation command (which is case sensitive and must be in lower case letters) then enter the number of degrees to rotate the label. For example, to rotate the label 45 degrees enter:</p> <pre>\rotation 45</pre> <p>To rotate the text and use LaTeX, the rotation command must be used first. For example:</p> <pre>\rotation 45 \latex Mole-fraction Al_2O_3</pre> <p>Rotates the text 45° and includes subscripts in the title Mole-fraction Al<sub>2</sub>O<sub>3</sub>.</p> <p>TEXT SIZE: <code>/.35/:</code> &lt;SIZE FOR THE LABEL&gt;</p> <p>A smaller size of the text may be necessary to fit the label text into the diagram. A default size is given using the latest size in adding label texts, or .35 if the command is called for the first time. A recommended size is e.g. 0.25.</p> <p> These changes to plot labels can also be manually edited in the <b>Console Results</b> window.</p>

## APPEND\_EXPERIMENTAL\_DATA

Add experimental data and text onto a calculated diagram. This is done by placing the experimental data and text on a formatted textual file (always having an extension of EXP) that is prepared outside of

Thermo-Calc software (Console Mode and Graphical Mode), according to the syntax of the DATAPLOT Graphical Language.

The picture generated from the data is superimposed on the ordinary graphical output from the postprocessor. Such an experimental data file (\*.EXP) may be created by an ordinary textual editor.

Another important usage of this command is to superimpose plots from several independent calculations. For this purpose, there is a command [MAKE\\_EXPERIMENTAL\\_DATAFILE](#) on page 199, which dumps a calculated diagram on an EXP file according to the DATAPLOT syntax. With the aid of a normal text editor, many such files may be merged together. Remember that you can only have one prologue section on each such EXP file.



Also see the *DATPLOT User Guide* included with this documentation set.

Syntax	APPEND_EXPERIMENTAL_DATA
Prompts	<p>USE EXPERIMENTAL DATA (Y OR N) /N/: &lt;Y OR N&gt;</p> <p>Specify whether the data from an experimental data file should be included in the next plot. If the answer is <code>c</code>, no experimental data are plotted.</p> <p>An <b>Open</b> window displays to specify the name of the file with the experimental data.</p>
	<p>PROLOGUE NUMBER: /0/: &lt;PROLOGUE NUMBER&gt;</p> <p>Select which prologue to use. In a prologue, you can, for example, give the scaling of an axis, the axis texts, and so on.</p> <p><input checked="" type="checkbox"/> By answering -1, a list of all prologues on the file is given; and by 0, no experimental data are appended.</p>
	<p>DATASET NUMBER(S) /-1/: &lt;DATASET NUMBER(S)&gt;</p> <p>Select from which dataset(s) data should be read. Several datasets may be given separated with commas or spaces. By answering -1, a list of all datasets on the file is given; and by 0, no experimental data are appended.</p>

## CHANGE\_LEGEND


When there is a legend in the diagram you can append constitution and/or ordering descriptions to the phase name.



[LIST\\_EQUILIBRIUM](#) on page 156 also displays `ORD` (ordered) or `DISORD` (disordered) (when available).



In some cases the legend only shows the phase name for a line when the [SET\\_LABEL\\_CURVE\\_OPTION](#) on page 209 option is set to F.

Syntax	CHANGE_LEGEND
Prompt	<p>SET SUFFIX FOR PHASE NAMES IN LEGEND? (ALL,NONE,CONSTITUTION,ORDERING) /NONE/:</p> <p>When you select <code>None</code> the legend includes the standard information about the phases.</p> <p>When you select <code>All</code> the Constitution description and the Ordering description (when there is ordering) are also included.</p> <p>When you select <code>Constitution</code>, this is added to the standard description.</p> <p>When you select <code>Ordering</code> and when there is ordering, this is added to the standard description.</p>
	<p> Also see <a href="#">About Legend Styles</a> on page 91 in the <i>Thermo-Calc User Guide</i> for examples of these labels.</p>

## DUMP\_DIAGRAM

After a Thermo-Calc graph is created (and displays with the PLOT\_DIAGRAM command) you can save (dump) a diagram to a file so you can quickly print it. It is similar to the PRINT\_DIAGRAM command.



Similar to [PRINT\\_DIAGRAM](#) on page 201, it does not matter what graphic device is set up for the graph, this command is always able to convert the graph shown on screen to the selected graphic format.

Syntax	DUMP_DIAGRAM
Prompt	<p>OUTPUT FORMAT /: &lt;FORMAT OR RETURN&gt;</p> <p>Specify an appropriate graphic format for dumping the graph or pressing &lt;Enter&gt; to accept the default format.</p>
	<p>A <b>Save</b> window opens if you have not specified a filename. Select a directory path and enter a <b>File name</b>. If a file with the specified name already exists, then you are prompted whether to overwrite the old file or not. The third argument of the command allows you to specify whether to overwrite (Y) the old file or not (N).</p>



After the printing process is finished, the temporarily set graphic device for conversion and printing is switched back to the one set by the command [SET\\_PLOT\\_FORMAT](#) on page 210, so that you can save the graph in file(s) using [PLOT\\_DIAGRAM](#) on page 200.

## ENTER\_SYMBOL

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

Functions or tables (with defined functions as values) can be entered in the POST module after a stepping or mapping calculation, for purposes of plotting such entered functions or tables as axis variables.

Within the POLY module, symbols are normally defined prior to an equilibrium calculation (enforced by a C\_E command), stepping calculation (enforced by the command [STEP\\_WITH\\_OPTIONS](#) on page 172) or mapping calculation (enforced by [MAP](#) on page 158). These can be entered after an equilibrium calculation; however, for defined functions, variable or tables, it requires using [EVALUATE\\_FUNCTIONS](#) on page 155 before showing the corresponding values in the calculated equilibrium state.


The symbols entered in the POST module are not saved in the currently-loaded POLY3 workspaces. Therefore, if you want to apply such symbols in other similar calculations for the same defined system, you must use the ENTER\_SYMBOL command prior to the STEPPING or MAPPING calculation in the POLY module.




Also see [ENTER\\_SYMBOL](#) on page 72 for the GIBBS Module.



See example 44 in the *Console Mode Examples Guide* for an example of using variables and functions.

Syntax	ENTER_SYMBOL
Prompt	<p>CONSTANT, VARIABLE, FUNCTION OR TABLE? /FUNCTION/: &lt;KEYWORD&gt;</p> <p>The Keyword can be specified as CONSTANT, VARIABLE, FUNCTION or TABLE.</p> <ul style="list-style-type: none"> <li>• <b>CONSTANTS</b> can only be entered once and is a means of using a name for a numeric value. For example, the value of 1 atmosphere in Pascal can be denoted by P0 after the command ENTER CONSTANT P0=101325. Defined constants can be used as values in condition assignments, for example, SET-COND P=P0.</li> <li>• <b>FUNCTIONS</b> are expressions of state variables or other functions. These expressions are saved, and whenever a function value is requested all functions are evaluated. The reason for this is that they may depend on each other.</li> <li>• <b>VARIABLES</b> are similar to functions because they can also be expressions of state variables. However, contrary to functions, they are only evaluated when they are entered or if they are explicitly named in an <a href="#">EVALUATE_FUNCTIONS</a> on page 155 command. It is possible to enter a variable with a new expression any time. This expression is evaluated directly and its value stored as the value of the variable. Defined variables can be used as values in the SET-CONDITION command.</li> <li>• <b>TABLES</b> are used for listing results from the STEP or MAP commands. A table consists of a list of any number of state variables, functions or variables. Defined tables can also be used in the post-processor POST.</li> </ul> <p> There is a special connection between tables and variables. If a variable is used in a table, it is evaluated for each line of the table in the TABULATE command or when the table is used in a plot.</p>
	<p>NAME: &lt;NAME OF THE SYMBOL&gt;</p> <p>Each symbol has a unique name that must start with a letter and can have maximum 8 characters.</p> <p>Legal characters include letters (either UPPER or lower case), digits and underscore _. Any other special character, such as parentheses ( and ), plus +, minus -, slash / or \, full stop (.), are illegal for symbol names.</p> <p>You can enter the symbol name and the value or function on the same line, these must be separated with an equal sign =, for example, TC=T-273.15 or T_C=T273.15 which stands for a definition of temperature in Celsius. Otherwise, these questions are asked.</p>



Syntax	ENTER_SYMBOL
	 For different types of symbol (constant, function, variable or table), the questions have different prompts.
	<p>FUNCTION: &lt;DEFINITION FOR A FUNCTION OR VARIABLE&gt;</p> <p><i>Functions</i> and <i>variables</i> are evaluated from an expression of state variables or other functions, constants or variables. The expression is a FORTRAN-like expression and operators +, -, *, = and ** can be used (** only with integer powers).</p> <p>Unary functions like LOG, LOG10, EXP, SIN, COS and ERF can also be used. An expression can be continued on more than one line. An expression should be terminated by a semicolon (;) or an empty line (by pressing &lt;Enter&gt; at the next prompt).</p> <p>Examples of function expressions:</p> <ul style="list-style-type: none"> <li>• GM(LIQUID) : The Gibbs energy of liquid per mole component</li> <li>• H.T/4.184: The heat capacity of the system in calories</li> <li>• ACR(CR) /X(FCC, CR) : The activity coefficient for Cr in FCC</li> <li>• T-273.15: The temperature in Celsius</li> </ul> <p>&amp;: &lt;CONTINUATION OF THE DEFINITION FOR THE SYMBOL&gt;</p> <p>The ampersand &amp; means that you can continue to write the function on the new line if one line is not enough for the function. If you finish the function press &lt;Enter&gt; again.</p>
	<p>VALUE: &lt;VALUE FOR A CONSTANT&gt;</p> <p>A <i>constant</i> can only be assigned a numeric value once.</p>
	<p>VALUE OR EXPRESSION: &lt;VALUE OF EXPRESSION FOR A VARIABLE&gt;</p> <p>A <i>variable</i> can be assigned a numeric value or an expression. An expression is evaluated immediately and discarded. Only the numeric value is kept. This gives a possibility to save a value between calculations with different conditions because all state variables and functions are evaluated for the new conditions.</p>
	<p>VARIABLE(S) : &lt;VARIABLE(S) IN A TABLE&gt;</p> <p>A <i>table</i> consists of a list of state variables or functions. One way to obtain results from a STEP command is through a table.</p> <p>Example:</p> <pre>ENTER TABLE K=T,X(LIQ,C),X(LIQ,CR),ACR(C)</pre> <p>Which means that the table called K contains four columns, i.e. the temperature, the mole</p>

Syntax	ENTER_SYMBOL
	<p>fractions of C and Cr in the LIQUID phase, and the activity of C.</p> <p>To show the temperature in Celsius in a table, give the command ENTER FUNCTION <math>TC=T-273</math>; and then use the symbol TC in the table.</p> <p>&amp; &lt;CONTINUATION OF THE DEFINITION FOR THE TABLE&gt;</p> <p>The ampersand &amp; means that you can continue to write the table on the new line if one line is not enough for the table. If you finish the table press &lt;Enter&gt; again.</p>

## FIND\_LINE


Identifies various property curves on a plotted property diagram (after a stepping calculation); it also works well in find stable phase regions on a phase diagram (after a mapping calculation).

Syntax	FIND_LINE
Prompts	<p>X COORDINATE /.484623611/: &lt;VALUE OF THE X COORDINATE&gt;</p> <p>Specify the value of the X coordinate where you want to find the details of property curve (or phase region).</p>
	<p>Y COORDINATE /.5153737962/: &lt;VALUE OF THE Y COORDINATE&gt;</p> <p>Specify the value of the Y coordinate where you want to find the details of property curve (or phase region).</p> <p>The POST module displays the identified property (for a property curve on a property diagram), or the identified stable phase-assemblage (for a phase region on a phase diagram).</p>

## LIST\_DATA\_TABLE

This command is used for listing various properties (i.e. the Y-axis variable on a property diagram) that change with an independent variable (i.e. the X-axis variable on a property diagram), which have already been defined in the POST module (and often are plotted on the **Console Results** window), but only after a STEP calculation.

The listing output can be either on screen or in a spreadsheet file in the MS Excel format (under specified file name with the default file extension of XLS), which can be further edited or used for graphical handling by opening the file (using the MS-Excel program) outside of the Thermo-Calc software system.

Syntax	LIST_DATA_TABLE
Prompt	<p>OUTPUT TO SCREEN OR FILE /SCREEN/: &lt;FILE NAME OR RETURN &gt;</p> <p>Specify a file name if you want to save on a spreadsheet file (in the MS Excel format, with the default extension of <code>XLS</code>) on which the already-defined properties on a property diagram (after a STEP calculation) is saved, or press &lt;Enter&gt; if want to see a simple textual table on screen (for the already-defined properties that change alone with an independent variable).</p> <p> This command only works for a property diagram after a stepping calculation but not for any phase diagram after a mapping calculation.</p>

## LIST\_PLOT\_SETTINGS

Syntax	LIST_PLOT_SETTINGS
	Lists the present values of most parameters specifying the type of diagram to be plotted.

## LIST\_SYMBOLS

For both the POLY and POST modules, list the definitions for all constants, functions, variables and tables.

In order to find the value of a function or variable, use [SHOW\\_VALUE on page 172](#) or [EVALUATE\\_FUNCTIONS on page 155](#). A table is tabulated with the TABULATE command.

Syntax	LIST_SYMBOLS
	The defined variables are listed up together with the defined functions, but variable names are followed by a percentage sign %.

## MAKE\_EXPERIMENTAL\_DATAFILE

Write the graphical information onto screen or a formatted text file (always having an extension of EXP) using the DATAPLOT graphical format. In order to merge two or more diagrams from separate calculations, you can write them out on files with this command, and then add/edit them together with a normal textual editor.




Also see the *DATPLOT User Guide* included with this documentation set.

Syntax	MAKE_EXPERIMENTAL_DATAFILE
Prompt	<p>OUTPUT TO SCREEN OR FILE /SCREEN/: &lt;NAME OF A FILE OR RETURN&gt;</p> <p>Specify the name of the desired file. Accept <code>SCREEN</code> (press &lt;Enter&gt;) for a list. Otherwise, a file name where the graphical information is written must be given here. The default file extension is <code>EXP</code> (under MS Windows) or <code>exp</code> (under Linux).</p>

## MODIFY\_LABEL\_TEXT

Move a label created with the command [ADD\\_LABEL\\_TEXT](#) on page 190 to another position, or replace its text with another one.

The label texts and the coordinates, either added by `ADD_LABEL_TEXT` command or modified by this command or manually edited on the Console Results window, are stored in the workspace, and can be saved onto an `*.EXP` file (through [MAKE\\_EXPERIMENTAL\\_DATAFILE](#) on the previous page).

Syntax	MODIFY_LABEL_TEXT
Prompts	<p>WHICH LABEL TO MODIFY? /#/ : &lt;NUMBER OF THE LABEL&gt;</p> <p>Before this prompt, all the labels created by the <code>ADD_LABEL_TEXT</code> command is listed with an identifying number. Specify the number of the label you want to modify. The default one (#) is the last added label.</p>
	<p>NEW X COORDINATE: /XXX/ : &lt;NEW X POSITION&gt;</p> <p>Specify the new X position. The previous X coordinate is displayed. Press &lt;Enter&gt; to accept.</p>
	<p>NEW Y COORDINATE: /YYY/ : &lt;NEW Y POSITION&gt;</p> <p>Specify the new Y position. The previous Y coordinate is displayed. Press &lt;Enter&gt; to accept.</p>
	<p>NEW TEXT /ABCDEFGH.../ : &lt;NEW LABELING TEXT&gt;</p> <p>Specify the new labeling text. The previous text is displayed. Press &lt;Enter&gt; to accept.</p> <div>  <p>The new label text must not be longer than the previous text.</p> </div>

## PLOT\_DIAGRAM

With this command, a calculated/plotted diagram is displayed if the default graphic device has already been defined by the [SET\\_PLOT\\_FORMAT](#) on page 210 command. It can also be saved onto a file.



The diagram axes must be set first.

The functionality of this command is shared in two ways:

- in `PLOT_DIAGRAM` for normal screen display and file saving and
- in [PRINT\\_DIAGRAM](#) below (under MS-Windows environment) for direct hard-copy printing.

Syntax	<code>PLOT_DIAGRAM</code>
Prompt	OUTPUT TO SCREEN OR FILE /SCREEN/: <NAME OF A FILE OR RETURN FOR SCREEN>
	<p>Specify the name of the desired file (Note that under Linux, the prompt is <code>PLOTFILE /SCREEN/</code>). Consequently, a file with a proper extension for the selected graphic format (set by the <code>SET_PLOT_FORMAT</code> command) is saved under the current working directory. If no extension is given in the file name, the default extension e.g. ps for Postscript portrait/landscape modes, P7 or p7 for HPGL landscape, P8 or p8 for HPGL portrait, etc.) is automatically given to the file name.</p> <p>If the default device is set (by the command <code>SET_PLOT_FORMAT</code>), you can either accept <code>SCREEN</code> to plot the graph in the Thermo-Calc Graph window on screen by pressing &lt;Enter&gt;, or save it on a file by giving a file name.</p>

## PRINT\_DIAGRAM

Syntax	<code>PRINT_DIAGRAM</code>
	<p>Print with high quality to a file after a Thermo-Calc graph is created (and is displayed with <a href="#">PLOT_DIAGRAM</a> on the previous page). It has the same function as the Print Plot option on the Console Results windows.</p>

## QUICK\_EXPERIMENTAL\_PLOT

This is similar to [APPEND\\_EXPERIMENTAL\\_DATA](#) on page 192 but can be used when there is no graphical information to be plotted in the POLY3 workspace. It defines a pair of axis, sets the axis labels to X and Y, and scales both X- and Y-axes between 0.0 and 1.0 unless a prologue is read from the DATAPLOT (\*.EXP) data file.



Also see the *DATPLOT User Guide* included with this documentation set.

Syntax	QUICK_EXPERIMENTAL_PLOT
Prompts	<p>PROLOGUE NUMBER: /0/: &lt;PROLOGUE NUMBER&gt;</p> <p>An <b>Open</b> window displays. Select the prologue to use. In a prologue, you can, for example, give the scaling of an axis, the axis texts, and so on. By answering -1, a list of all prologues on the file is given; and with 0, no experimental data are appended.</p>
	<p>DATASET NUMBER(S) /-1/: &lt;DATASET NUMBER(S)&gt;</p> <p>Select from which dataset(s) data should be read. Several datasets may be given separated with commas or spaces. By answering -1, a list of all datasets on the file is given; and with 0, no experimental data are appended.</p>

## REINITIATE\_PLOT\_SETTINGS

All parameters describing the diagram are given default values.

Syntax	REINITIATE_PLOT_SETTINGS
	All plot settings made in the POST module are deleted, and it returns to the initial settings when the POST module is entered.

## RESTORE\_PHASE\_IN\_PLOT

Restores a phase previously suspended from the plot with [SUSPEND\\_PHASE\\_IN\\_PLOT](#) on page 216. It works only after at least one phase is suspended.

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

## SELECT\_PLOT

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

Syntax	SELECT_PLOT
Prompt	<p>PLOT &lt;N/NEW&gt;</p> <p>Where N is a positive integer. Enter the number of the plot that is selected in the <b>Console Results</b> window (in the currently selected <b>Results</b> tab). If a plot with that number does not exist, it is created.</p> <p>The default parameter value is <b>NEW</b>. If this is entered, then a new plot is created. Create a new plot can also be done by pressing Ctrl+Shift+T.</p>

## SET\_AXIS\_LENGTH

Change the real length of an axis in inches. The default number of tic-marks on an axis is 10 when the relative length is 1. The number and units per tic-mark must be a multiple of 1, 2 or 5 to obtain a reasonable scaling of an axis.

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

## SET\_AXIS\_PLOT\_STATUS

Specify whether the axis title texts and axis label texts are to be plotted or not on a diagram. It does not work for the axis lines and tic-marks. If you want to plot a diagram without tic-marks, use [SET\\_TIC\\_TYPE](#) on page 215 first.


This can be used to merge different diagrams on a pen-plotter or to obtain the diagram faster. The default status is that all the set axes are to be plotted.

Syntax	SET_AXIS_PLOT_STATUS
Prompt	<p>AXIS PLOT (Y OR N) /Y/: (Y OR N)</p> <p>Specify to plot axis texts (Y) or no (N).</p>

## SET\_AXIS\_TEXT\_STATUS

Change the axis text from the automatic text given by the axis specification to a text.

Syntax	SET_AXIS_TEXT_STATUS
Prompts	<p>AXIS (X, Y OR Z) : &lt;NAME OF AN AXIS&gt;</p> <p>Specify which axis text status to change.</p>
	<p>AUTOMATIC AXIS TEXT (Y OR N) /N/: &lt;Y OR N&gt;</p> <p>Specify if automatic axis text is to be used (Y) or (N). If you answer N, enter axis text.</p>
	<p>AXIS TEXT: &lt;ENTER AXIS TEXT&gt;</p> <p>You can enter simple text, use LaTeX, rotate the text, as well as adjust the font size.</p>

Syntax	SET_AXIS_TEXT_STATUS
	 Also see <a href="#">ADD_LABEL_TEXT</a> on page 190.

## SET\_AXIS\_TYPE

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

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

## SET\_COLOR

Some devices support colours or line thickness. With this command, select different colors or line types on some types of information on a diagram.




This command can fail if a chosen device does not support colors or line thickness.

This command gives four sequential prompts (i.e. Text and axis, Invariant equilibria, Tie-lines, and All other lines), with the Keyword and default option (both listed below). Depending on if the switched-on graphic device (by the SET\_PLOT\_FORMAT command) supports colors or line types, the POST automatically switches on the appropriate Keyword.

Syntax	SET_COLOR
Prompt	<p>TEXT AND AXIS KEYWORD /DEFAULT OPTION/ &lt;RETURN OR NEW OPTION&gt;</p> <p>INVARIANT EQUILIBRIA KEYWORD /DEFAULT OPTION/: &lt;RETURN OR NEW OPTION&gt;</p> <p>TIE-LINES COLOR KEYWORD /DEFAULT OPTION/: &lt;RETURN OR NEW OPTION&gt;</p> <p>KEYWORD OF ALL OTHER LINES /DEFAULT OPTION/: &lt;RETURN OR NEW OPTION&gt;</p> <p>This is usually for the solubility lines.</p>



Syntax	SET_COLOR
	 The <code>Keyword</code> is either <code>Color</code> or <code>LineType</code> , depending on if color or line type is supported by the switched-on graphic device (by the <a href="#">SET_PLOT_FORMAT on page 210</a> command); the POST module <i>automatically</i> switches on the appropriate <code>Keyword</code> .

## Color Options

The options for `Color` are:

BACKGROUND	BLUE	PURPLE	GRAY
FOREGROUND (default)	YELLOW	GOLD4	ORANGERED3
RED (default for invariant equilibria)	MAGENTA	TURQUOISE4	MAROON
GREEN (default for tie lines)	CYAN	PINK	PLUM
	SIENNA	OLIVEDRAB	SEAGREEN
	ORANGE1	CORAL1	USERDEF

## LineType Options

The options for `LineType` are:

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

## SET\_CORNER\_TEXT

Adds text to the corners on a plotted diagram. Normally, you can write such texts as a subtitle.

The primary database (not the appended ones) used in calculations and the calculated conditions are automatically plotted at the upper-left corner as a part of the header on all plotted diagram. Unless the plotting option `WRITE CONDITIONS` is switched off by the command [SET\\_PLOT\\_OPTIONS on page 211](#),

the calculated conditions are always written on plotted diagrams; and only when the plotting option PLOT HEADER is switched off by the command SET\_PLOT\_OPTION, the used database also always appear. Under such circumstance, avoid writing texts at the UPPER\_LEFT corners.

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

## SET\_DIAGRAM\_AXIS

Specify an axis variable for a plot or a listing. To be able to plot a diagram, at least two axis variables (x and y) must be specified. In the Thermo-Calc Console Mode, three axes (x, y and z) can be specified for a diagram.



The axis variables in the plot can be different from the number of axis used for the mapping.

If you want to plot a phase diagram with tie-lines in the plane after a MAP calculation, then the composition axis must be mole-fraction or weight-fraction, or mole-percent or weight-percent of one specific component. You must not use the stable variable  $x(\text{comp})$  or  $w(\text{comp})$  even if that is what you used when calculating the diagram, because that only gives one side of the two-phase region. It may be sufficient to indicate that mole-fraction is the same as the stable variable  $x(*, \text{comp})$ , and weight-fraction is the same as the stable variable  $w(*, \text{comp})$ .

If you plot a phase diagram where the tie-lines are not in the plane after a MAP calculation, then mole-fraction and  $x(\text{comp})$  are identical.

When you plot a property diagram after a STEP calculation and want a composition axis variable, you should normally use  $x(\text{comp})$  and not mole-fraction.

The axis must have exactly the same number of columns, or one axis must have one column. In the first case the columns are plotted matching them one by one; in the latter all columns on one axis is plotted against the single column. For example, you can have the temperature on one axis and the amount of

each phase on the other. The amount of each phase is the state variable  $NP(*)$  in mole fraction or  $BPW(*)$  for mass fractions of phases.

Automatic diagram axis: The POST module can set automatic diagram axis identical to those used in the [MAP on page 158](#) command.

If the state variable  $x(\text{comp})$  is used in a MAP calculation, then mole-fraction of the component is used as diagram axis; if a potential or some other state variables are used, then that is used as a diagram axis.

After a STEP calculation, automatic diagram axis is not set as there is only one axis used in the calculation.

Syntax	SET_DIAGRAM_AXIS
	<p>AXIS (X, Y OR Z) : &lt;AXIS NAME&gt;</p> <p>Specify which axis (X or Y or Z) to set with a variable.</p>
Prompts	<p>VARIABLE TYPE: &lt;VARIABLE NAME&gt;</p> <p>Specify a variable for the chosen axis here.</p> <p>The valid variables are:</p> <ul style="list-style-type: none"> <li>• TEMPERATURE-CELSIUS as temperature in oC</li> <li>• TEMPERATURE as temperature in K</li> <li>• PRESSURE as pressure in Pa</li> <li>• ACTIVITY for a component</li> <li>• LNACTIVITY for a component [ln(ACR(component))]</li> <li>• MOLE-FRACTION for a component</li> <li>• MOLE-PERCENT for a component</li> <li>• WEIGHT-FRACTION for a component</li> <li>• WEIGHT-PERCENT for a component</li> <li>• NONE to clear the axis</li> <li>• Any valid state variable including those with wildcards, e.g. <math>NP(*)</math> or <math>x(*, \text{component})</math>. Due to the use of wildcard * in such a state variable, the program asks for a column number.</li> <li>• Any entered function or variable.</li> <li>• Any entered table.</li> </ul>
	<p>If you specify an entered table as the variable, then you are given these prompts:</p> <p>FOR COMPONENT: &lt;COMPONENT NAME&gt;</p>

Syntax	SET_DIAGRAM_AXIS
	When an activity, mole or weight fraction or percent of a component shall be plotted, the component name must be supplied here.
	<p>COLUMN NUMBER: &lt;COLUMN NUMBER(S)&gt;</p> <p>Specify the column number(s) in the chosen table that are to be plotted onto the earlier specified axis. For example:</p> <ul style="list-style-type: none"> <li>• 1 for column 1</li> <li>• 2, 3 for columns 2 and 3</li> <li>• 2, 3 &gt;5 for column 2,3 and all columns above column 5</li> <li>• * for all columns</li> </ul>

## SET\_DIAGRAM\_TYPE

Choose the diagram type as perpendicular plot or triangular plot (Gibbs triangle, especially for ternary systems). The default is with a perpendicular axes.

For phase diagrams of ternary or pseudo-ternary systems, it is usually need to plot isothermal sections as triangular grams. If desired, all lines outside the region limited by a line joining the end points of the X- and Y-axis is removed.



In order to create a 3D-plot file (in the VRML format, \*.WRL) for a tetrahedron diagram, this command in the sequence SET\_DIAGRAM\_TYPE N Y should be used first.

Syntax	SET_DIAGRAM_TYPE
Prompts	<p>TRIANGULAR DIAGRAM (Y OR N) /N/: &lt;Y OR N&gt;</p> <p>Specify a triangular plot Y. Otherwise (by pressing &lt;Enter&gt; to accept N), perpendicular axis is set and this command is terminated. By default, perpendicular diagrams have (almost) the same scaling on both axes.</p>
	<p>CREATE TETRAHEDRON VRML FILE (Y OR N) /N/: &lt;Y OR N&gt;</p> <p>If a triangular plot is not selected (at the above prompt), answer Y in case a tetrahedron diagram is used to generate VRML (*.WRL) file by sequentially using the CREATE_3D_PLOTFILE command.</p>
	<p>PLOT 3:RD AXIS (Y OR N) /N/: &lt;Y OR N&gt;</p> <p>If a triangular plot is selected, specify if a 3rd axis (by answering Y here), connecting the end points of the X- and Y-axes, is plotted.</p>


Syntax	SET_DIAGRAM_TYPE
	CLIP ALONG 3:RD AXIS (Y OR N) /N/: <Y OR N>
	If a triangular plot is selected, all lines outside the region limited by a line joining the end points of the X- and Y-axis are removed by answering Yes (Y).

## SET\_FONT

Select the font to use for labels and numbers when plotting the diagram under the currently selected graphic device ([SET\\_PLOT\\_FORMAT](#) on the next page). For some devices there may be other fonts available and these are selected by the SET\_PLOT\_FORMAT command.

Syntax	SET_FONT
Prompts	<p>SELECT FONTNUMBER /1/: &lt;#&gt;</p> <p>Specify an available font number # as the default font for the current graphic device, or accept the font number 1 by pressing &lt;Enter&gt;. By typing a question mark ? here, the program lists the available fonts under the currently selected graphic device.</p>
	<p>FONT SIZE /.34/: &lt;##&gt;</p> <p>The size of the chosen font is specified. A value around 0.34 is recommended.</p>

## SET\_INTERACTIVE\_MODE


Syntax	SET_INTERACTIVE_MODE
	<p>Resets the input and output units to their initial values, i.e. keyboard and screen.</p> <p> Remember to add this as the last command to your MACRO files, in order to stop execution of the command file in the POST module. It has no meaning in interactive mode.</p>

## SET\_LABEL\_CURVE\_OPTION

Identify the curves drawn in the post-processor by marking each curve with a digit and then list the meaning of these digits beside the plot.



The number of digits can be quite large in some cases. If so, use the SET\_FONT command and reduce the font size; usually, 0.2 is sufficient.

Syntax	SET_LABEL_CURVE_OPTION
Prompt	CURVE LABEL OPTION (A, B, C, D, E, F OR N) /A/: <OPTION>
	<p>The options:</p> <ul style="list-style-type: none"> <li>• A: List stable phases along line</li> <li>• B: As A but curves with same fix phase have same number</li> <li>• C: List axis quantities</li> <li>• D: As C but curves with same quantities have same number</li> <li>• E: As B with changing colors</li> <li>• F: As D with changing colors</li> <li>• N: No labels</li> </ul> <p>This question is rather cryptic but usually the option B or E is good for phase diagrams (after a MAP command) and option D or F for property diagrams (after a STEP command). Those interested can try out the option A and C by themselves.</p> <p> Option B or E lists the fixed phases along each curve, whereas option D or F gives the axis variables used along each curve. E provides varied colors for different stable-phase curves on phase diagrams (after a MAP command); F provides varied colors for different property curves on property diagrams (after a STEP command). The option N (NONE) disables all curve labels and lists.</p> <p>If, for example, you use T (temperature in K) as the variable axis in a STEP command and then plot the amount of stable phases (with <a href="#">SET_DIAGRAM_AXIS on page 206</a> Y NP ( * ) ) on the Y-axis versus T-C on the X-axis, then the list may have lines like:</p> <pre>1: T-273.15, NP (LIQUID) 2: T-273.15, NP (FCC_A1)</pre> <p>This means that for curve 1 the X-axis is T-273.15 (the same for all curves, of course) and NP (LIQUID) on the Y-axis. Curve 2 has the same X-axis but NP (FCC_A1) on the Y-axis.</p>

## SET\_PLOT\_FORMAT

Set the format of the graphical output to different graphical devices. The default graphic device is normally for screen output (number 22 - TCUNITE Driver). Legacy devices can still be used (1 for Windows and 9 for XWindow for Linux). This default graphic device value may also be altered with [SET\\_PLOT\\_ENVIRONMENT on page 243](#) in the system monitor or by your TC.INI file.

Syntax	SET_PLOT_FORMAT
Prompt	<p>GRAPHIC DEVICE NUMBER /#/: &lt;NUMBER OF THE DEVICE&gt;</p> <p>Specify a graphic device number. Depending on the hardware, different plot formats (graphic devices) may be available. These are listed online by giving a question mark ?.</p> <p>For some formats there can be additional sub-prompts, asking for if using (YES) or not using (NO) the fonts available for the chosen format, and if YES for further specifications, e.g. font type and size.</p>

## SET\_PLOT\_OPTIONS

You are prompted for and can toggle on (Y) or off (N) the plotting of some options on all subsequently generated diagrams.

For the `Always initiate POST on re-entering prompt`, the default is Y which implies that the POST module automatically reinitiates whenever the POLY3 workspace is changed upon re-entering. If answered N the same diagram axis variables are kept even if the workspaces in the POLY module are read from or written to an \*.POLY3 file. The N answer is useful when there are several sets of \*.POLY3 files with the same calculation but for different sets of model parameters.

For the `Always solid line prompt`, the default answer is N which means that the POST module plots solid lines for stable phases but dashed lines for metastable phases. This is normally for plotting property diagram after a STEPPING calculation; however, when there is a metastable extrapolation in a phase region on a phase diagram after a MAPPING calculation, this is also enforced. When the alternative answer Y is chosen, all the lines are always plotted in solid lines.

Syntax	SET_PLOT_OPTIONS
Prompts	<p>PLOT HEADER /Y/: &lt;Y OR N&gt;</p> <p>Toggle the plotting of the Thermo-Calc header text above a diagram.</p>
	<p>PLOT LOGO /Y/: &lt;Y OR N&gt;</p> <p>Toggle the plotting of the Thermo-Calc logotype at the lower-left corner of a diagram.</p>
	<p>PLOT FOOTER /Y/: &lt;Y OR N&gt;</p> <p>Toggle the plotting of the footer identifier text at the right margin of a diagram.</p>
	<p>WHITE-CONTOURED-PS-CHARS /Y/: &lt;Y OR N&gt;</p> <p>This makes it possible to write PostScript characters in white contoured status.</p>
	<p>PLOT REMOTE EXPONENT(S) /Y/: &lt;Y OR N&gt;</p>

Syntax	SET_PLOT_OPTIONS
	This sets (Y) or removes (N) the plotting of the remote exponent on the axis.
	<p>PLOT SYMBOLS AT NODE POINTS /0/: &lt;#&gt;</p> <p>This makes it possible to plot symbols at the node points on plotted lines on a diagram.</p>
	<p>SYMBOL SIZE /.1/: &lt;.#&gt;</p> <p>Set the size of symbols which are plotted at the node points.</p>
	<p>WRITE CONDITION? /Y/: &lt;Y OR N&gt;</p> <p>The initial equilibrium conditions for the current calculations are automatically plotted at the upper-left corner as a part of the header. With this option switched off (by answering N), it makes possible to not write the calculated conditions on a plotted diagram.</p>
	<p>WRITE DATABASE NAME? /Y/: &lt;Y OR N&gt;</p> <p>Primary database (not the appended ones) used in the current calculations are automatically plotted at the upper-left corner as a part of the header. With this option switched off (by answering N), it makes possible to not write the database name on a plotted diagram.</p>
	<p>ALWAYS INITIATE POST ON RE-ENTERING: /Y/: &lt;Y OR N&gt;</p> <p>Y lets the POST module automatically reinitiate whenever the POLY3 workspaces are changed upon re-entering. If answered N, the same diagram axis variables are kept even if the workspaces in the POLY module is read from or written to an *.POLY3 file. Answering N is useful when there are several sets of *.POLY3 files with the same calculation but for different set of model parameters.</p>
	<p>ALWAYS SOLID LINE: /N/: &lt;Y OR N&gt;</p> <p>N allows the POST module to plot solid lines for stable phases but dashed lines for metastable phases. This is normally for plotting property diagram after a STEPPING calculation; however, when there is a metastable extrapolation in a phase region on a phase diagram after a MAPPING calculation, this is also enforced. When answered Y all the lines are always plotted in solid lines.</p>

## SET\_PLOT\_SIZE

Change the size of the diagram by specifying a global plot size (as a relative scaling factor). The default value of the relative scaling factor is 1, while the real size of the plotted diagram depends on what output device is chosen with [SET\\_PLOT\\_FORMAT](#) on page 210. The default plot size (corresponding to the default global plot size 1) is adjusted to the chosen device.



Syntax	SET_PLOT_SIZE
Prompt	<p>GLOBAL PLOT SIZE /1/: &lt;RELATIVE SCALING FACTOR&gt;</p> <p>Enter the relative scaling factor as a numerical number (e.g. 0.5, 0.8, 1.0, 1.5, etc.). By pressing &lt;Enter&gt;, the default relative scaling factor (1) is accepted.</p>

## SET\_PREFIX\_SCALING

Set the prefix scaling of remote exponents with certain powers (default is 3), by taking as argument with an `axis name` and a YES, or NO, or an integer number # (as the powers for the remote exponents):

NO switches off its action.

YES arranges the prefix scaling so that the axis scaling is done with the remote exponents being powers of three, i.e. ..., -6, -3, 0, 3, 6, ...

# sets the remote exponents as being powers of #.

Syntax	SET_PREFIX_SCALING
Prompt	<p>AXIS (X, Y OR Z): &lt;NAME OF AN AXIS&gt;</p> <p>Specify which axis is to have a prefix scaling.</p>
	<p>USE PREFIX SCALING /Y/: (Y OR N OR #)</p> <p>Answer either Y or N or an integer number as described above.</p>

## SET\_RASTER\_STATUS

Plot a raster (i.e. with gridlines on both axis directions) in the diagram. The default status is no raster plotted.

Syntax	SET_RASTER_STATUS
Prompt	<p>RASTER PLOT (Y OR N) /N/: &lt;Y OR N&gt;</p> <p>Enable (Y) or disable (N) the raster plot.</p>

## SET\_REFERENCE\_STATE

The reference state for a component is important when calculating activities, chemical potentials and enthalpies. After calculating with [STEP\\_WITH\\_OPTIONS on page 172](#) or [MAP on page 158](#), the reference state for a component can also be changed for plotting various properties of the component in the entire system or in a specific phase by using this command. Afterwards, you can set diagram axes as chemical potential or activity quantities with the R suffix, i.e. MUR(comp), MUR(comp,ph), ACR(comp), ACR(comp,ph) or their common logarithms [e.g. LNACR(comp,ph)].

Syntax	SET_REFERENCE_STATE
Prompts	<p>COMPONENT: &lt;NAME OF THE COMPONENT&gt;</p> <p>The name of the component must be given.</p>
	<p>REFERENCE STATE: &lt;NAME OF A PHASE USED AS THE NEW REFERENCE STATE&gt;</p> <p>The Name of a phase, that must be either ENTERED, DORMANT or SUSPENDED, is given here. The component must, of course, be a constituent of this phase.</p> <p>A subtle problem is that if the component exists in several species in the phase, for example, oxygen as O, O2 and O3 in a gas. Normally, you would like to have the most stable species as reference state of oxygen, i.e. O2 in this case. When setting the reference state, a one-time calculation is made for the Gibbs energy. This is for all possible states with the pure component phase at the current temperature and the command selects the most stable one as the reference state.</p>
	<p>TEMPERATURE /*/: &lt;REFERENCE TEMPERATURE&gt;</p> <p>Select the temperature (in K) for the reference state. The value * means the current temperature is used for the calculation.</p>
	<p>PRESSURE /1E5/: &lt;REFERENCE PRESSURE&gt;</p> <p>Select the pressure (in Pa) for the reference state. The value * means the current pressure is used for the calculation.</p>

## SET\_SCALING\_STATUS

When an axis variable is selected by [SET\\_DIAGRAM\\_AXIS](#) on [page 206](#), the scaling status for the axis is always set to automatic scaling. By this command, choose between manual or automatic scaling on a specified axis. If manual scaling is chosen, specify a minimum and a maximum value. Manual scaling can be used to magnify interesting parts of a diagram.

Syntax	SET_SCALING_STATUS
Prompts	<p>AXIS (X, Y OR Z): &lt;NAME OF AN AXIS&gt;</p> <p>Specify which axis that you want to set the scaling status.</p>
	<p>AUTOMATIC SCALING (Y OR N) /N/: &lt;Y OR N&gt;</p> <p>Choose between automatic (Y) and manual scaling (N). For manual scaling specify these parameters:</p>
	<p>MIN VALUE: &lt;MINIMUM VALUE&gt;</p> <p>The minimum value at the start point of the specified axis.</p>
	<p>MAX VALUE: &lt;MAXIMUM VALUE&gt;</p>

Syntax	SET_SCALING_STATUS
	The maximum value at the end point of the specified axis.

## SET\_TIC\_TYPE

Change the drawing of the axis tics. You may alter the placement of tic marks on the axis, e.g. inside or outside or no tic marks. The size of tic marks cannot be altered by this command, but these are adjusted based on the selected graphic device and the defined relative scaling factor (global plot size).

Syntax	SET_TIC_TYPE
Prompt	<p>TIC TYPE /1/: &lt;1 OR -1 OR 0&gt;</p> <p>The tic type 1 is default, i.e. the tics are drawn outside the diagram. -1 means that the tics are inside the diagram and 0 means no tics.</p>



## SET\_TIELINE\_STATUS

If the tie-lines are in the plane of the calculation, you can select to plot the tie-lines in two-phase fields with this command.

Syntax	SET_TIELINE_STATUS
Prompt	<p>PLOTTING EVERY TIE-LINE NO /0/: &lt;NUMBER OF TIE-LINES&gt;</p> <p>The tie-lines plotted are not equally spaced by the graphics software. Instead, you can select to plot a subset of the calculated tie-lines, i.e. every one (1), every second (2), every three (3), etc. By accepting the default value 0, no tie-line is plotted.</p>

## SET\_TITLE

Specify a title that displays on all listed tables and plotted diagrams from the POST module in the same run of Console Mode.

Syntax	SET_TITLE
Prompt	<p>TITLE: &lt;TITLE&gt;</p> <p>Enter the title you want to appear on all tabulation or graphic outputs.</p> <div>  <p>There is a maximum length of about 60 characters for the title. You can enter simple text, use LaTeX, rotate the text, as well as adjust the font size.</p> </div> <div>  <p>Also see <a href="#">ADD_LABEL_TEXT</a> on page 190.</p> </div>

## SET\_TRUE\_MANUAL\_SCALING

The tic-marks on the axes are normally placed in even intervals using the whole axis length. The scaling routine adjusts the given minimum and maximum values slightly to accomplish this. If such an automatic adjustment behaviour is unwanted, it can be avoided by using this command (followed by a message showing the TRUE MANUAL SCALING set for a specific axis).

The command works like a toggle. To reset the automatic scaling behaviour, repeat the command a second time for that specific axis (followed by a message saying the SEMI\_MANUAL SCALING set for the specific axis).

Syntax	SET_TRUE_MANUAL_SCALING
Prompt	<p>AXIS (X, Y OR Z): &lt;NAME OF AN AXIS&gt;</p> <p>Specify which axis (X or Y or Z) you want to toggle between automatic adjustments or avoid the adjustment of the given maximum and minimum values.</p>

## SUSPEND\_PHASE\_IN\_PLOT

Specify that lines originating from the presence of a certain phase shall not be plotted on a diagram. If you want to bring the suspended phase back to the diagram, use [RESTORE\\_PHASE\\_IN\\_PLOT](#) on page 202.

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

## TABULATE

For any entered table, this command gives a table of values from equilibria calculated with a STEP command. It works only for a table that is entered in either the POLY or POST module.



Unlike the TAB module's command (also called [TABULATE](#) on page 253) it is not possible to plot columns from the tabulated tables. For this use normal POST commands.

Syntax	TABULATE
Prompts	<p>NAME: &lt;NAME OF A TABLE ENTERED IN EITHER POLY OR POST&gt;</p> <p>Specify a table name that is entered in either the POLY or POST module.</p>
	<p>OUTPUT ON SCREEN OR FILE /SCREEN/: &lt;FILE NAME OR RETURN&gt;</p> <p>Specify a file name if you want to save on a file the table values along the defined STEP calculation, or press &lt;Enter&gt; if want to see the table values displayed.</p>

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## POTENTIAL\_DIAGRAM Module

In this section:

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<i>POTENTIAL_DIAGRAM</i> .....	218
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## POTENTIAL\_DIAGRAM

The POTENTIAL\_DIAGRAM module (short name, the POTENTIAL module) is a potential phase diagram calculation module.

If you have a metal-oxide/sulphide-gas interaction system, you might want to calculate a so-called potential phase diagram given certain temperature and pressure. A potential diagram uses the activities of two major species in the gaseous mixture phase as mapping variables. The activities (that is, the fugacities at 1 bar) of these two species are typically set as the X- and Y-axis when the diagram is plotted. The phase relations between the gaseous mixture and various metal forms, metal-oxides, metal-sulphides, or other metal-bearing solids, are represented by different fields controlled by these two potential quantities.

To enter the module, at the SYS prompt type `GOTO_MODULE POTENTIAL`.

There are no commands for this module. Follow the prompts and see [About Potential Diagrams on page 158](#) in the *Thermo-Calc User Guide* for details about how to calculate using potential diagrams.



See example 35 in the *Console Mode Examples Guide*.

Syntax	POTENTIAL_DIAGRAM
Prompts	<p>DATABASE: /POT/</p> <p>Press &lt;Enter&gt; and the program lists the available databases. Type one of the database names and press &lt;Enter&gt; to select. The following default elements are then based on the chosen database.</p> <p>MATRIX_ELEMENT: /FE/</p> <p>FIRST_POTENTIAL_SPECIES: /S1O2/</p> <p>SECOND_POTENTIAL_SPECIES: /O2/</p> <p>TEMPERATURE: /1000/</p>

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## POURBAIX\_DIAGRAM Commands



Also search the online help or see the Pourbaix diagrams educational material and the *Thermo-Calc User Guide*.

In this section:

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<i>POURBAIX_DIAGRAM Commands</i> .....	<a href="#">220</a>
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## POURBAIX\_DIAGRAM Commands



Also search the online help for additional information in other guides.



See examples TCEX40 and TCEX53 in the *Console Mode Examples Guide*.

After you enter the POURBAIX\_DIAGRAM module, you are prompted with the following:

```
NEED ANY INSTRUCTION ON THE POURBAIX MODULE? /N/:Y
```

If you answer `Y` the following notes are displayed.

- The Pourbaix diagram is actually a calculated equilibrium phase diagram mapped and plotted with the independently-varied electropotential (Eh, as defined with regard to the standard hydrogen electrode as its reference) and acidity (pH), that represents all the equilibrated phase boundaries among aqueous solution, gaseous mixture, and various primary and secondary solids (modelled as either complex solution or simple stoichiometric phases) in a certain multicomponent heterogeneous interaction system, under a defined T-P condition and a specific initial bulk composition (which is, by default, always set as 1 kg of water dissolving a specified amount of metals/alloys and other acids/alkalines/salts).
- At least one database is required that contains an AQUEOUS solution phase (with thermodynamic data for water and various aqueous solutes), that shall be selected from TCAQ (PAQ) or AQS (PAQS) [which use the SIT Model or the Complete Revised HKF Model, respectively] within the Thermo-Calc database spectrum, or be chosen from an appropriate USER-specified database (it must be in the Thermo-Calc TDB format).
- Due to the restrictions of aqueous solution model used within Thermo-Calc, such a database must be designed in the same format as in the default TCAQ (PAQ) or AQS (PAQS) for AQUEOUS solution phase. Among others, one should keep in mind the following regulations:
  - The ELECTRON is defined as a special element (ZE) and as the only constituent in its reference phase REFERENCE\_ELECTRODE (for determining the electropotential that is defined as Eh with the standard hydrogen electrode as the reference), but it is not defined as an aqueous species;
  - The vacancy (VA) is unnecessary for AQUEOUS solution phase and it should be avoided in the definition of phase-constituents in the AQUEOUS phase;
- The AQUEOUS solution phase should always be defined as a constitutional solution phase, implying that all the aqueous solution species must be included in a single site,



rather than in two or multiple sublattices.

- Beside the AQUEOUS solution phase, there shall exist a GAS mixture phase containing at least H<sub>2</sub>O, O<sub>2</sub> and H<sub>2</sub>; and for multicomponent systems, normally there shall also contain some solid (stoichiometric or solution) phases. Of course, if desired, you could also choose to calculate and generate a Pourbaix diagram without considering the GAS mixture phase entirely; however, such a plot is not really a complete Pourbaix diagram, due to the fact that thermodynamically-stable phase boundaries between the AQUEOUS solution phase and GAS mixture phase will then not be calculated at all!
- All the required thermodynamic data for calculations of Pourbaix diagrams or other diagrams must be retrieved either from one (Single) database which consists of an AQUEOUS solution phase, a Gaseous mixture phase, a REF\_ELECTRODE phase, and some SOLID phases (being solutions and/or stoichiometric compounds; for primary metals/alloys and for secondary products formed from heterogeneous chemical/electrochemical interactions, or from several (Multiple) databases that respectively contain various solutions/compounds (as listed above).

Such databases suitable for calculations of aqueous-bearing heterogeneous interaction systems can be those default-prompted ones [i.e., in the Single-Database case, the PAQ or PAQS; and in the Multiple-Database case, the TCAQ or AQS as primarily-switched database, plus the SSUBx as firstly-appended one and the SSOLx as secondly-appended one if it is necessary; even more databases can be appended). Of course, you could also choose to append required data from other appropriate databases (such as TCFE, TCSLD, TCNI/TTNi, TCAL/TTAI, TCMG/TTMg, TTZr, TCMP, SLAG, etc.) for Gaseous mixture phase and for various solid solution and stoichiometric compound phases. Furthermore, an experienced user can also utilize his/her own USER-specified databases in various cases.

- The current advanced POURBAIX-Module has been designed and developed in an efficient and effective way that it only requires the user to just answer some simple and necessary questions, rather than to go through basic modules (i.e., TDB, GES5, POLY3 and POST) and type the ordinary command-lines. Beside the default plotted Pourbaix diagram, it also allows the user to easily and quickly plot many different properties of the system, stable phases and aqueous species, varied along the calculated phase boundaries for the same defined heterogeneous interaction system. Moreover, it permits the user to directly change some plotting settings and manipulate all kinds of plotted diagrams.
- The current advanced POURBAIX-Module has been extended so that it is additionally able to directly perform a normal STEPPING calculation (varied with a specified independent variable) and to easily generate various types of property diagrams, for the same heterogeneous interaction system that has been defined in a previous POURBAIX or TDB-GES5-PLOY3-POST calculation.

## Pause Options

After this information is displayed, you are prompted:

ENFORCE A PAUSE AFTER PLOTTING WHEN RUNNING A MACRO? /N/:

If you answer Y the following options are displayed.

1. START A COMPLETELY NEW POURBAIX DIAGRAM CALCULATION
2. OPEN AN OLD FILE & PLOT OTHER PROPERTY DIAGRAMS
3. OPEN AN OLD FILE & MAKE ANOTHER POURBAIX CALCULATION
4. OPEN AN OLD FILE & MAKE ANOTHER STEPPING CALCULATION

## Option 1: Start a completely new POURBAIX diagram calculation

Make a completely new POURBAIX diagram calculation and automatically plot a pH-Eh diagram. i.e., define a new chemical system; specify the T-P-X conditions; calculate the initial equilibria; perform the pH-Eh mapping calculation; plot pH-Eh & various property diagrams.

CONSIDER THE GAS PHASE IN CALCULATING A POURBAIX DIAGRAM? /Y/

USE SINGLE DATABASE? /Y/:

COMBINED DATABASE: /PAQ2/:

DEFINE A CHEMICAL SYSTEM AND ITS INITIAL BULK COMPOSITION:

Normally a POURBAIX diagram and related equilibrium property in a heterogeneous interaction system are calculated under a certain bulk composition which is usually 1 kg of water with defined amounts of dissolving solute substances. The solutes may either be completely dissolved into the aqueous solution, or be partially dissolved and simultaneously form some solid phases.

CHEMICAL SYSTEM (ELEMENTS):

Default defined elements (solvent H<sub>2</sub>O): 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 H<sub>2</sub>O

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 CO<sub>2</sub> CoCl<sub>3</sub> Fe<sub>0.93</sub>S NaSO<sub>4</sub>-1 H<sub>2</sub>SO<sub>4</sub>

Mass of Water (weight) = 1 kg

## Option 2: Open an old file and plot other property diagrams

Open an existing POLY3 file created by POURBAIX Module (from a previous POURBAIX calculation Option 1 or 3 or a previous STEPPING calculation Option 4), and just selectively plot other property diagrams. i.e., open the old GES and POLY3 workspaces; plot pH-Eh or various property diagrams.

FILE NAME /POURBAIX/

X-AXIS VARIABLE: /PH/:

Y-AXIS VARIABLE: /EH/:

CHANGE AXIS TYPE? /N/:

ZOOM IN? /N/:

CHANGE CURVE-LABEL OPTION FOR THE DIAGRAM? /N/:

ADD LABEL-TEXTS ONTO THE SPECIFIED DIAGRAM? /N/:

CHANGE THE SUBTITLE OF THE DIAGRAM? /N/:

CHANGE AXIS-TEXTS? /N/:

FURTHER REFINE THE DIAGRAM IN POST MODULE? /N/:

HARD COPY OF THE DIAGRAM? /N/:

SAVE X-Y COORDINATES OF CURVE ON TEXT FILE? /N/:

MODIFY THE DIAGRAM? /N/:

ANY MORE DIAGRAM? /N/:

### Option 3: Open an old file and make another POURBAIX calculation

Open an existing POLY3 file created by POURBAIX Module and make another POURBAIX diagram calculation i.e., open the old GES and POLY3 workspaces; adopt the defined chemical system; modify the T-P-X conditions; calculate the initial equilibria; perform the pH-Eh mapping calculation; plot pH-Eh & various property diagrams.

CONSIDER THE GAS PHASE IN CALCULATING A POURBAIX DIAGRAM? /Y/:

FILE NAME /C:\USERS\AMANDA\DOCUME~1\POURBA~1.POL/:

ENFORCE GLOBAL MINIMIZATION TECHNIQUE IN CALCULATIONS? /N/:

SAVE ALL FUNCTIONS, VARIABLES AND TABLES IN POLY3 FILE? /Y/:

SET NUMERICAL LIMITS? /N/:

SET CALCULATING PARAMETERS:

LIST OF DEFAULT AND PRE-DEFINED CALCULATION CONDITIONS:

UNITS: T IN K, P IN PASCAL, B(H<sub>2</sub>O) IN GRAM, N(ELEM) IN MOLE

T=298.15, P=1E5, B(H<sub>2</sub>O)=1000, N(H+1)=0, N(ZE)=0

DEGREES OF FREEDOM 0

CONFIRM DEFINED CONDITIONS? /Y/:

### Additional Information About Option 3

The default definitions of the Eh and pH quantities in the advanced POURBAIX-Module (and in the ordinary TDB-GES-POLY calculation routines) should ALWAYS be as below:

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

where RNF is the Faraday constant (96485.309 C/mol), and AH<sub>2</sub>O is the molecular weight of H<sub>2</sub>O (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)\*AH<sub>2</sub>O] 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 H<sub>2</sub>O, 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, H<sub>2</sub>S). The reference state for the H<sub>2</sub>O component must always be defined as the solvent species H<sub>2</sub>O in the AQUEOUS solution phase under the current temperature (\*) and 100000 Pascal (i.e., 1 bar). The reference states for the H+1 and ZE components are by default set as their SER.

Various conventional properties of aqueous solute species I are converted in the following manners:

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

where YH<sub>2</sub>O [i.e., Y(AQUEOUS, H<sub>2</sub>O)] and Y(AQUEOUS, I) are the site-fractions of solvent H<sub>2</sub>O and solute species I.

#### LIST THE DEFINED AXIS-VARIABLES:

```
Axis No 1: LNACR(H+1)Min: -34.532525Max: 2.3025851 Inc: 0.8
Axis No 2: MUR(ZE)    Min: -150000    Max: 200000    Inc: 7718.85
```

**NOTE:** The default settings (listed above) for two mapping variables [in terms of lnACR(H+1) and MUR(ZE), and their minimum/maximum values and increment steps] are covering the following pH-Eh ranges/steps:

```
pH: 0.00 -> 14.00, at a step of 0.35
Eh: -1.55 -> 2.07, at a step of 0.08 (V)
```

The maximum pH limit has been calculated precisely and determined automatically by the POURBAIX-Module, as a function of the temperature-pressure conditions and initial bulk compositions of the current defined interaction system.

```
ACCEPT THE DEFAULT SETTINGS FOR TWO MAPPING VARIABLES? /Y/:
ANY MISSING PHASE BOUNDARY YOU COULD POSSIBLY THINK OF? /N/:
CHANGE THE PH/EH STEPS FOR SMOOTHER CURVES? /N/:
ZOOM IN? /N/:
CHANGE CURVE-LABEL OPTION FOR THE DIAGRAM? /N/:
ADD LABEL-TEXTS ONTO THE POURBAIX DIAGRAM? /N/:
CHANGE THE SUBTITLE OF THE DIAGRAM? /N/:
CHANGE AXIS-TEXTS? /N/:
FURTHER REFINE THE DIAGRAM IN POST MODULE? /N/:
HARD COPY OF THE DIAGRAM? /N/:
SAVE X-Y COORDINATES OF CURVE ON TEXT FILE? /N/:
MODIFY THE DIAGRAM? /N/:
ANY MORE DIAGRAM? /N/:
```

## Option 4: Open an old file and make another STEPPING calculation

Open an existing POLY3 file created by POURBAIX Module (from a previous POURBAIX calculation Option 1 or 3 or a previous STEPPING calculation Option 4), and make a normal STEPPING calculation. i.e., open the old GES and POLY3 workspaces; adopt the defined chemical system; specify one of the T-P-X conditions as the stepping variable; calculate the initial equilibria; perform the stepping calculation; plot various property diagrams.

Because of that in a STEPPING calculation will change some system definitions in a POURBAIX-type POLY3 file, it is highly advisable to make a backup of the existing POURBAIX-type POLY3 file (which you are going to open in this STEPPING calculation) before you proceed the further steps; otherwise, the structure of the loaded POLY3 file will be alternated by the option "4", and consequently the existing POLY3 file may be not suitable for other POURBAIX-type calculation any longer. Therefore, if you have not done so, you should make the copy right now!

However, a POLY3 file which is modified by this option can be further used for another STEPPING calculation inside the POURBAIX Module (by a repeated Option 4) or in normal POLY3 Module.

```
FILE NAME /C:\USERS\AMANDA\DOCUME~1\POURBA~1.POL/:
ENFORCE GLOBAL MINIMIZATION TECHNIQUE IN CALCULATIONS? /N/:
SAVE ALL FUNCTIONS, VARIABLES AND TABLES IN POLY3 FILE? /Y/:
SET NUMERICAL LIMITS? /N/:

SET CALCULATING PARAMETERS:
List of Default and Pre-defined Calculation Conditions:
-----
Units: T in K, P in Pascal, B(H2O) in gram, N(ELEM) in mole
-----
T=298.15, P=1E5, B(H2O)=1000, N(H+1)=0, N(ZE)=0
DEGREES OF FREEDOM 0
FURTHER MODIFY SYSTEM DEFINITIONS & CONDITIONS IN POLY3 MODULE? /N/:
CONFIRM DEFINED CONDITIONS AS THE STARTING POINT? /Y/:
```

The following parameters are suitable for a STEPPING calculation for the defined aqueous-bearing system. Choose one of them as the stepping variable:

```
T Temperature (C)
P Pressure (bar)
pH Acidity
Eh Electronic Potential (V)
N(Comp) Mole of One Component
```

where "Comp" is the name of a specific component as listed below. One should not use any key component (H2O or H+1 or ZE) as such a stepping variable, because of that their compositional definitions and variations are determined by the AQUEOUS solution phase in the POURBAIX Module.

An interacting component defined as an element (such as Fe or Na or Cl) can be selected as a stepping variable.

However, if you want to make a stepping calculation with a non-element chemical formula (such as NaCl or CaS<sub>2</sub>) as the stepping variable, one must have made some necessary modifications in the POLY3 Module, before reaching this point, by conducting some POLY3 commands as given below (as an example for the system Fe-Na-Cl-H-O):

```
POLY_3: def-component H2O H+1 ZE Fe NaCl Cl
POLY_3: set-ref-state H2O AQUEOUS * 1E5
POLY_3: set-ref-state ZE REF_ELEC * 1E5
POLY_3: change-status phase REF-ELEC=SUSPEND
POLY_3: set-cond b(H2O)=1000 n(H+1)=0 n(ZE)=0
POLY_3: set-cond P=1E5 T=298.15**
POLY_3: set-cond n(Fe)=1E-3 n(Cl)=0 n(NaCl)=3 **
```

\*\* Here the P-T-n(Fe) conditions can be set as what you wanted, while the initial n(NaCl) value must be set as between its minimum and maximum values that you are interested in. Later on, it will be prompted for specifying the n(NaCl) Min-Max-Step values of the stepping calculation.

```
STEPPING VARIABLE: /T/:
MINIMUM TEMPERATURE (C) /15/:
MAXIMUM TEMPERATURE (C) /35/:
INCREMENT IN TEMPERATURE (C) /1/:
CHANGE AXIS TYPE? /N/:
ZOOM IN? /N/:
CHANGE CURVE-LABEL OPTION FOR THE DIAGRAM? /N/:
ADD LABEL-TEXTS ONTO THE SPECIFIED DIAGRAM? /N/:
CHANGE THE SUBTITLE OF THE DIAGRAM? /N/:
CHANGE AXIS-TEXTS? /N/:
FURTHER REFINE THE DIAGRAM IN POST MODULE? /N/:
HARD COPY OF THE DIAGRAM? /N/:
SAVE X-Y COORDINATES OF CURVE ON TEXT FILE? /N/:
MODIFY THE DIAGRAM? /N/:
ANY MORE DIAGRAM? /N/:
```

---

## REACTOR\_SIMULATOR\_3 Commands

In this section:

---

<i>CREATE_DIVIDERS</i> .....	229
<i>CREATE_PIPES</i> .....	229
<i>CREATE_STAGE_BOXES</i> .....	230
<i>EXECUTE_POLY3_COMMAND</i> .....	231
<i>LIST_RECORDS</i> .....	231
<i>READ_WORKSPACE</i> .....	232
<i>SAVE_WORKSPACE</i> .....	232
<i>START_SIMULATION</i> .....	233



## CREATE\_DIVIDERS

Define the segment boundaries and the ways on how to distribute phases between various segments and to split the feeds of heat and mass.

Syntax	CREATE_DIVIDERS
Prompts	<p>NUMBER OF DIVIDERS /4/: &lt;THE NUMBER OF DIVIDERS&gt;</p> <p>Specify the number of dividers (boundaries between various segments) in the reactor. It is normally the segment number plus one: for example, if the stage box number is defined as 4, the divider number should be defined as 5.</p>
	<p>NUMBER OF OUTPUTS FOR DIVIDER # /3/: &lt;THE NUMBER OF OUTPUTS&gt;</p> <p>Specify the number of outputs for a specific divider #.</p>
	<p>PERCENT OF INPUT TO OUTPUT 1 /100/: &lt;PERCENT OF INPUT&gt;</p> <p>Define the percentage of input to the output 1 in the current divider #.</p>
	<p>PERCENT OF INPUT TO OUTPUT ## /100/: &lt;PERCENT(S) OF INPUT(S)&gt;</p> <p>Define the percentages of inputs to the outputs ## in the current divider #. It is repeated till the last output is specified.</p>

## CREATE\_PIPES

Define the pipes between various segments and the ways on how the mass and heat transport between the surroundings (with the record number as 0) and the reactor, among various segments in the reactor, and along various dividers (segment boundaries in the reactor).

Syntax	CREATE_PIPES
Prompts	<p>FROM RECORD: &lt;A RECORD NUMBER&gt;</p> <p>Specify a record number. If there are four segments in the reactor, these records are available:</p> <ul style="list-style-type: none"> <li>• 0 surroundings</li> <li>• 1-4 stage boxes (segments)</li> <li>• 5-9 dividers (segment boundaries)</li> </ul>
	<p>PIPE TO RECORD: &lt;ANOTHER RECORD NUMBER&gt;</p> <p>Specify another record number to which the mass or heat flows from the current record (specified above). Before this prompt, a message shown on the screen indicates what kind of mass or heat flow (according to the definitions of stage boxes and dividers, which have already been created prior to this command) should be specified in the pipe. This is</p>

Syntax	CREATE_PIPES
	repeated for all inputs and/or outputs for mass and/or heat in current record.

## CREATE\_STAGE\_BOXES

Create several reaction stages as boxes (segments), where the you define the feed in either mass input and initial temperature or heat input from surroundings, as well as the mass out and initial temperature in each of the segments.

Syntax	CREATE_STAGE_BOXES
Prompts	<p>NUMBER OF STAGE BOXES /4/: &lt;THE NUMBER OF STAGE BOXES&gt;</p> <p>Specify the number of stage boxes in the reactor. Then define the feed of mass and/or energy (from surroundings to) the rector.</p>
	<p>GIVE FEED TO SYSTEM: &lt;FEED&gt;</p> <p>One feed (of mass or heat) to the reactor must be specified here. Two types of feeds can be used:</p> <ul style="list-style-type: none"> <li>• As input amount of heat (enthalpy): H=Value.</li> <li>• As input amount of specific species or element and its initial temperature: N(SPECIES)=Value, Input temperature (in one line, or the input temperature in the next prompt).</li> </ul>
	INPUT TEMPERATURE /298.15/: <INPUT TEMPERATURE>
	<p>GIVE FEED TO SYSTEM: &lt;FEED&gt;</p> <p>Specify other feeds (mass or energy) to the reactor. Press &lt;Enter&gt; to finish the feed inputs, and then:</p> <p>GIVE FOR STAGE BOX #</p> <p>Now start to define the type of stage box (segment is specifically numbered as #), and to specify a guess of initial temperature and an output for each phase in the segment.</p>
	<p>TYPE OF BOX /EQUILIBRIUM/: &lt;TYPE OF BOX&gt;</p> <p>Only the EQUILIBRIUM type is allowed. Press &lt;Enter&gt; to accept it.</p>
	<p>IS THE STAGE HEAT CONTROLLED? /Y/: &lt;YES OR NO&gt;</p> <p>Y means the current segment is heat controlled.</p>
	<p>INITIAL GUESS OF TEMPERATURE? /1000/: &lt;INITIAL TEMPERATURE&gt;</p> <p>Give a guess of initial temperature (in K) for the current segment; press &lt;Enter&gt; to accept</p>

Syntax	CREATE_STAGE_BOXES
	the default.
	<p>GIVE INITIAL AMOUNT: &lt;INITIAL AMOUNT OF MASS OR HEAT&gt;</p> <p>The initial amount of mass and/or heat in the current segment can be specified here. Two types of initial amount can be used:</p> <ul style="list-style-type: none"> <li>• As initial amount of heat (enthalpy): H=Value.</li> <li>• As initial amount of specific species or element and its initial temperature: N(SPECIES)=Value, Input temperature (in one line, or the input temperature in the next prompt).</li> </ul>
	INPUT TEMPERATURE /298.15/: <INPUT TEMPERATURE>
	<p>GIVE INITIAL AMOUNT: &lt;INITIAL AMOUNT OF MASS OR HEAT&gt;</p> <p>Specify initial amount (mass or energy) in the current segment. Press &lt;Enter&gt; to finish the initial amount inputs, and then this message displays:</p> <p>Each phase may have a separate output, give these</p> <p>Now start to define the output for each phase.</p>
	<p>PHASE NAME /REST/: &lt;NAME OF PHASE&gt;</p> <p>Specify a phase that has a separate output, e.g. GAS; by pressing &lt;Enter&gt; to accept that all REST phases do not have separate outputs. Then the program asks for further definitions of all the other segments (one by one), repeating some of the above questions, till the last segment in the reactor is defined.</p>

## EXECUTE\_POLY3\_COMMAND

Syntax	EXECUTE_POLY3_COMMAND
	To directly use all kinds of POLY commands inside the REACTOR module. Any legal <i>POLY_3 Commands</i> on page 117 can be entered.

## LIST\_RECORDS

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

## READ\_WORKSPACE

The REACTOR workspace (along with the related POLY3 and GIBBS workspaces) and the simulated results from the SIMULATE command can be read by this command from a binary file where they must be saved with [SAVE\\_WORKSPACE](#) below. The \*.RCT file is not printable.

Syntax	READ_WORKSPACE
Options	<p><b>File name:</b> The name of a saved *.RCT file where the REACTOR and POLY3/GIBBS workspaces shall be read from must be specified. You do not need to type the extension if it is the default .RCT, otherwise type the whole *.RCT file name.</p> <p>An <b>Open</b> window displays if a file name is not given after the command or its path is incorrect, so that the path (in the <b>Look in</b> field) and <b>File name</b> can be specified. The <b>Files of type</b> (i.e. RCT) cannot be changed.</p>

## SAVE\_WORKSPACE

The REACTOR (and POLY3/GIBBS) workspaces are saved on a file with this command. In the GIBBS workspace, all thermochemical data are stored. In the POLY3 workspace, all thermochemical data, all conditions, changed status, entered symbols, etc., are stored. In the REACTOR workspace, all definitions of multi-stage steady-state reactor and its distribution coefficients are saved, together with the GIBBS and POLY3 workspaces. After a SAVE command, you can always return to the state when you issued the SAVE command by giving a READ command.

After saving the REACTOR (and POLY3/GIBBS) workspaces on a file, you can leave the program and at a later time READ the file and continue from the saved state.



A START\_SIMULATE command automatically saves on the work file with the most lately specified name. To avoid destroying the simulated results, do not SAVE after a START\_SIMULATE command is enforced, similar to that you should not SAVE after a STEP or MAP command! You may append several results by START\_SIMULATE without destroying the previous results but SAVE erases them all.

Syntax	SAVE_WORKSPACE
	<p>FILE NAME</p> <p>A file name must be specified. The default extension of the RCT file is .RCT, while or any other extension as required.</p>
	<p>A <b>Save</b> window displays if a file name is not given after the command, so that the path (in the <b>Save in</b> field) and <b>File name</b> can be specified. The <b>Files of type</b> (i.e. RCT) cannot be changed. If there is already a file with the same file name under the directory a warning message displays. Click <b>OK</b> to overwrite the current REACTOR (and POLY3/GIBBS) workspaces onto the existing *.RCT file. Click <b>Cancel</b> to return to the REACTOR module. You</p>

Syntax	SAVE_WORKSPACE
	can use the SAVE command with an unspecified name (i.e. through SAVE , , , command-sequence) to save the REACTOR (and POLY3/GIBBS) workspaces.

## START\_SIMULATION

Start the reactor simulation, and list the results for all iterations. The output for each iteration consists of the conditions set in each segment, and you can also select some state variables to list. After each loop, the temperatures in all segments are listed.

Syntax	START_SIMULATION
Prompts	<p>MAX NUMBER OF LOOPS /10/: &lt;THE MAX NUMBER OF LOOPS&gt;</p> <p>Give the max number of loops. The REACTOR module repeats the reactor simulation until this loop number is reached.</p>
	<p>OUTPUT TO SCREEN OR FILE /SCREEN/: &lt;FILE NAME OR RETURN&gt;</p> <p>Decide on either listing simulation results on the screen (by pressing &lt;Enter&gt;) or saving them on an experimental file (with the default extension .EXP).</p> <p><input checked="" type="checkbox"/> The conditions in each segment are not saved in the file, only on the screen.</p>
	<p>OUTPUT VARIABLES /T BP(\$)/: &lt;VARIABLE NAME(S)&gt;</p> <p>Specify the variable name(s) that is also listed on the screen together with the conditions in each segment, or in the output experimental file.</p>

### Example Output

For a four-stage reactor, the output at a certain iteration may look like this:



```
H=-991745.1, P=100000, N(C)=2.8468936, N(N)=6.78399966E-4, N(O)=3.8171615,
N(SI)=1.77031
DEGREE OF FREEDOM 0
BP(GAS)=43.464341, BP(C1SI1_BETA)=25.175981, BP(C_S)=8.1588099,
BP(QUARTZ_S3)=68.193896
1.78803E+03
BP(GAS)=61.971213, BP(C1SI1_BETA)=38.144346, BP(QUARTZ_L)=66.230717 2.06569E+03
BP(GAS)=67.66262, BP(C1SI1_BETA)=35.480983, BP(QUARTZ_L)=58.219292
2.08691E+03
BP(GAS)=71.23129, BP(SI_L)=22.471787
2.20831E+03
```

---

H=-924751,87, P=100000, N(C)=2.0594558, N(N)=5.17999978E-4, N(O)=4.0142358,  
N(SI)=2.7551438  
DEGREE OF FREEDOM 0  
BP(GAS)=43.464341, BP(C1SI1\_BETA)=25.175981, BP(C\_S)=8.1588098,  
BP(QUARTZ\_S3)=68.193896  
1.78803E+03  
BP(GAS)=61.971213, BP(C1SI1\_BETA)=38.144346, BP(QUARTZ\_L)=66.230717 2.06569E+03  
BP(GAS)=67.66262, BP(C1SI1\_BETA)=35.480983, BP(QUARTZ\_L)=58.219292  
2.08691E+03  
BP(GAS)=71.23129, BP(SI\_L)=22.471787  
2.20831E+03  
H=-813239., P=100000, N(C)=1.6592668, N(N)=3.59999988E-4, N(O)=3.7549293,  
N(SI)=2.896635  
DEGREE OF FREEDOM 0  
BP(GAS)=43.464341, BP(C1SI1\_BETA)=25.175981, BP(C\_S)=8.1588098,  
BP(QUARTZ\_S3)=68.193896  
1.78803E+03  
BP(GAS)=61.971213, BP(C1SI1\_BETA)=38.144346, BP(QUARTZ\_L)=66.230717 2.06569E+03  
BP(GAS)=67.66262, BP(C1SI1\_BETA)=35.480983, BP(QUARTZ\_L)=58.219292  
2.08691E+03  
BP(GAS)=71.23129, BP(SI\_L)=22.471787  
2.20831E+03  
H=7374.6403, P=100000, N(C)=8.84911857E-1, N(N)=1.99999996E-4, N(O)=1.9379203,N  
(SI)=1.853872  
DEGREE OF FREEDOM 0  
BP(GAS)=43.464341, BP(C1SI1\_BETA)=25.175982, BP(C\_S)=8.1588097,  
BP(QUARTZ\_S3)=68.193896  
1.78803E+03  
BP(GAS)=61.971213, BP(C1SI1\_BETA)=38.144346, BP(QUARTZ\_L)=66.230717 2.06569E+03  
BP(GAS)=67.66262, BP(C1SI1\_BETA)=35.480983, BP(QUARTZ\_L)=58.219292  
2.08691E+03  
BP(GAS)=71.23129, BP(SI\_L)=22.471787  
2.20831E+03  
10 1788.03 2065.69 2086.91 2208.31 0.00 0.00 0.00

---

## SCHEIL Commands

-  Search the online help or see the *Thermo-Calc User Guide* included with this PDF documentation set for details about how to calculate using Scheil either in Graphical Mode (the Scheil Calculator) and Console Mode (the wizard Scheil module).
-  If you also have a license for the Diffusion Module (DICTRA), you can import a previously calculated Scheil segregation profile into the software using the command INPUT\_SCHEIL\_PROFILE. Search the online help or see the *Diffusion Module (DICTRA) Command Reference Guide*.


In this section:

---

<i>BCC_TO_FCC_TRANSFORMATION</i> .....	<i>236</i>
<i>EVALUATE_SEGREGATION_PROFILE</i> .....	<i>236</i>
<i>GLOBAL_MINIMIZATION</i> .....	<i>236</i>
<i>LIQUID_PHASE_NAME</i> .....	<i>236</i>
<i>SAVE_FILE_NAME</i> .....	<i>237</i>
<i>START_WIZARD</i> .....	<i>237</i>
<i>TEMPERATURE_STEP</i> .....	<i>238</i>
<i>TERMINATION_CRITERIA</i> .....	<i>238</i>


## BCC\_TO\_FCC\_TRANSFORMATION

Use this command for the Scheil module to allow transformations in the solidified part of the alloy caused by each of the components specified to be Fast Diffuser. It is recommended that you only select this for steels.

Syntax	BCC_TO_FCC_TRANSFORMATION
Prompt	ALLOW BCC  FCC ? /N/ The default is N. Enter Y to allow transformations.

## EVALUATE\_SEGREGATION\_PROFILE

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

Syntax	EVALUATE_SEGREGATION_PROFILE
Prompt	EVALUATE SEGREGATION PROFILE? /N/   If answer Y, then this feature is not supported with back diffusion.
	NUMBER OF GRID POINTS /100/  Segregation profile is dumped to a file XF.TXT in the current directory.

## GLOBAL\_MINIMIZATION

Use this command for the Scheil module to use global minimization.



Also see the POLY commands topic [ADVANCED\\_OPTIONS Descriptions on page 120](#) for information about that GLOBAL\_MINIMIZATION command.

Syntax	GLOBAL_MINIMIZATION
Prompt	USE GLOBAL MINIMIZATION? /N/  If Y, the Global Minimization is done when possible (depending on the conditions setting), and a Global Minimization test is performed when an equilibrium is reached. This costs more computer time but the calculations are more robust. If N the Global Minimization is not used to reach the equilibrium.

## LIQUID\_PHASE\_NAME

Use this command for the Scheil module to use the liquid phase name from the database definitions or enter another phase name.



Syntax	LIQUID_PHASE_NAME
Prompt	LIQUID PHASE NAME /DEFAULT/ Default selects the liquid phase from the database definitions, otherwise enter a phase name.

## SAVE\_FILE\_NAME

Use this command for the Scheil module to save the file. The files get the console number added to this name, e.g. 005.->Scheil\_006.poly3 and Scheil\_segregation\_profile.txt).

Syntax	SAVE_FILE_NAME
Prompt	Name of files to be saved, poly3 and segregation profiles.

## START\_WIZARD

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

This wizard walks you through a basic Scheil simulation. You are prompted for settings including the major element or alloy, composition input in mass (weight) percent, the alloying elements, the temperature, fast diffusing components, and whether any phase should have a miscibility gap check.

Use the other commands to make changes to settings that are not included in this wizard.

- BCC\_TO\_FCC\_TRANSFORMATION
- EVALUATE\_SEGREGATION\_PROFILE
- GLOBAL\_MINIMIZATION
- LIQUID\_PHASE\_NAME
- SAVE\_FILE\_NAME
- STORED\_COMPOSITION\_TYPE
- TEMPERATURE\_STEP
- TERMINATION\_CRITERIA

Syntax	START_WIZARD
Prompt	DATABASE /<DEFAULT>/: MAJOR ELEMENT OR ALLOY: COMPOSITION INPUT IN MASS (WEIGHT) PERCENT? /Y/: 1ST ALLOYING ELEMENT:CR 10 C 1 NEXT ALLOYING ELEMENT: TEMPERATURE (C) /2000/: FAST DIFFUSING COMPONENTS: /NONE/:C SHOULD ANY PHASE HAVE A MISCIBILITY GAP CHECK? /N/:

## TEMPERATURE\_STEP

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

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

## TERMINATION\_CRITERIA

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

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

---

## SYSTEM\_UTILITIES Commands

In this section:

---

<i>ABOUT</i> .....	240
<i>CLOSE_FILE</i> .....	240
<i>DISPLAY_LICENSE_INFO</i> .....	240
<i>HP_CALCULATOR</i> .....	240
<i>OPEN_FILE</i> .....	241
<i>SET_COMMAND_UNITS</i> .....	241
<i>SET_ECHO</i> .....	242
<i>SET_INTERACTIVE_MODE</i> .....	242
<i>SET_LOG_FILE</i> .....	242
<i>SET_PLOT_ENVIRONMENT</i> .....	243
<i>SET_TC_OPTIONS</i> .....	243
<i>STOP_ON_ERROR</i> .....	244

## ABOUT

Syntax	ABOUT
	Lists basic information about the development history and ownership of the Thermo-Calc software and its components.

## CLOSE\_FILE

Close an opened text file.

Syntax	CLOSE_FILE
Prompt	UNIT NUMBER: <UNIT NUMBER> A unit number given in an OPEN_FILE command must be specified.

## DISPLAY\_LICENSE\_INFO

Use this command to launch a license diagnostics program implemented in the SYS module. It detects the license information for the Thermo-Calc installations on the current client computer (and on the connected license server), and lists the details, including the current status of available license file and all its included license features for the current installation(s), as well as the Safenet Environment Variables and detailed Local (Client) Information, on screen or into a textual file (\*.TXT).

This is useful for a list of license details, and to obtain basic technical support by sending the \*.TXT file to [support@thermocalc.se](mailto:support@thermocalc.se). If you are running a network client installation of Thermo-Calc, you can see how many of the client example licenses that are currently checked out and how many of them are left. You can also see which clients computers it is that have checked these client example licenses out.

Syntax	DISPLAY_LICENSE_INFO
Prompt	OUTPUT TO SCREEN OR FILE /SCREEN/: <MYLICENSEINFO.TXT> Press <Enter> to display a list of license information or into a *.TXT file under a specific file name which can later on be opened and edited by any basic text editor.

## HP\_CALCULATOR

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

Syntax	HP_CALCULATOR
	<p>Available OPCODEs (HPC codes) are listed by entering the command HELP.</p> <p>Use the BACK command to quit the HP_CALCULATOR and go back to the SYS module.</p> <p>Input are numbers, + - * / and ^ and OPCODEs. Several numbers and operations can be given on one line. The content of the X register is displayed after each operation.</p> <p>For example, to compute <math>2 * \text{EXP}(1.5 * 3 - 30000 / (8 * 1273))</math>, you should input the following:  30000 8/1273/chs 1.5 3 ^ + exp 2 *</p>

## OPEN\_FILE

A text file is opened for use in other commands where a unit number is necessary. The program automatically assigns a unit number.

Syntax	OPEN_FILE
Prompt	<p>FILE NAME: &lt;FILE NAME&gt;</p> <p>A legal file name must be specified.</p>

## SET\_COMMAND\_UNITS


This command is useful for reading inputs already prepared by a textual editor on a file. Such inputs can be a table of values or a large number of parameters. The file must be opened with [OPEN\\_FILE](#) above.




The first two lines of an input file are skipped before any input is read.

Syntax	SET_COMMAND_UNIT
Prompt	<p>INPUT UNIT NUMBER /5/: &lt;INPUT UNIT NUMBER&gt;</p> <p>Specify the input unit number returned from an OPEN_FILE command. The next command is taken from the file connected to this unit number. The last command on such a file must be EXIT or SET_INTERACTIVE when you are in POLY, POST or SYS module, in order to go back to read input from the keyboard. The default value is the current input unit.</p> <p>OUTPUT UNIT NUMBER /6/: &lt;OUTPUT UNIT NAME&gt;</p> <p>Specify the output unit number returned from an OPEN_FILE command.</p>

## SET\_ECHO

Syntax	SET_ECHO
	<p>Add this command at the beginning of a Console Mode MACRO *.TCM file (or to the primary MACRO file on the top level if any sub-level(s) of MACRO files are used).</p> <p>Automatically displays on screen the complete details of various commands in all the sequential operations in the software, that are enforced according to the MACRO file(s).</p> <p> This command is not applicable if MACRO files are not used.</p>

## SET\_INTERACTIVE\_MODE

Syntax	SET_INTERACTIVE_MODE
	<p>Resets the input and output units to their initial values, i.e. keyboard and screen.</p> <p> Remember to add this as the last command to your MACRO files, in order to stop execution of the command file in the POST module. It has no meaning in interactive mode.</p>

## SET\_LOG\_FILE

Use it to save, in a basic text file, everything typed in the Thermo-Calc software. When having problems executing a command sequence, this command can be used to save the command typed onto a log file. The manager can then check what the problem might be.

This command also makes the system echo the full command for all commands typed. This feature is useful when demonstrating the system since the abbreviated commands are often difficult.

The saved log file can then be edited as a MACRO file by using a basic text editor. This is useful to run the MACRO file(s) for similar calculations (the same system but slightly varied temperature-pressure-composition conditions), or run the example MACRO files.

Syntax	SET_LOG_FILE
Prompt	<p>A <b>Save</b> window opens to specify a file name for the *.LOG file, so that the path (in the <b>Save in</b> field) and <b>File name</b> can be specified. If an *.LOG file with the same name exists in the current working directory, it is overwritten. The <b>Files of type</b> (i.e. LOG) cannot be changed. Click <b>Save</b> or <b>Cancel</b> as applicable.</p>

## SET\_PLOT\_ENVIRONMENT

Allows you, preferably in the initiation file tc.ini, to set the plot devices you normally have access to as this can vary for different Thermo-Calc installations.



This command must be terminated with an empty line or two commas.

Syntax	SET_PLOT_ENVIRONMENT
Prompts	<p>DEFAULT PLOTDEVICE NUMBER /DEFAULT NUMBER/: &lt;DEVICE NUMBER&gt;</p> <p>The number given is unique for each type of graphical device. For plotting various types of Thermo-Calc graphs on screen, the default graphical device number should normally be selected. A question mark ? gives you a list of all available graphical devices used in the Thermo-Calc Console Mode.</p>
	<p>PSEUDO FILE NAME: &lt;PSEUDO-FILE NAME&gt;</p> <p>The name given here is a symbol which can be used to refer to a physical graphics device when asked for graphical output file.</p>
	<p>PLOTDEVICE NUMBER /1/: &lt;DEVICE NUMBER&gt;</p> <p>The number that specifies the type of graphical device.</p>
	<p>PLOT FILE NAME: &lt;FILE NAME OR PRINTER NAME&gt;</p> <p>The name of the graphical device on system level (name of file or printer).</p> <p><b>Example</b></p> <pre>SET_PLOT_ENVIRONMENT 1 lasp 5 a0tr,,</pre> <p>This example sets the default plot device number to 1, and defines an alias named <code>lasp</code> with plot device 5 and connected to a printer named <code>a0tr</code>.</p>

## SET\_TC\_OPTIONS

Predefine the default values of three general Thermo-Calc options for performing all the sequential single-points, stepping and mapping calculations.

Syntax	SET_TC_OPTIONS
Prompts	<p>USE_GLOBAL_MINIMIZATION /YES/: &lt;Y OR N&gt;</p> <p>If Y, it is done when possible (depending on the conditions setting), and a Global Minimization test is performed when an equilibrium is reached. This costs more computer time but the calculations are more robust. For N Global Minimization is not used to reach the equilibrium.</p>
	<p>GLOBAL_TEST_INTERVAL /0/: &lt;AN INTEGER VALUE&gt;</p> <p>The integer number determines how often the Global Minimization should be used during calculations with <a href="#">STEP_WITH_OPTIONS</a> on page 172 and <a href="#">MAP</a> on page 158. If it is set to 0 (zero), the recommended global test interval is used: i.e. every tenth step and at each phase change during STEP calculations, and only at node points during MAP calculations. Any other positive integer number, n, suggests it performs Global Minimization tests at every nth step during STEP and MAP calculations. Of course, the Global Minimization test is always carried out at a phase change or a node point. The Thermo-Calc Console Mode is initially configured with 0 (zero) as the default value, but such a configuration for the default value can be changed by this option.</p>
	<p>AUTOMATICALLY_ADD_INITIAL_EQUILIBRIA /YES/: &lt;Y OR N&gt;</p> <p>When <a href="#">ADD_INITIAL_EQUILIBRIUM</a> on page 119 is not used before a MAP calculation, a mesh of INITIAL_EQUILIBRIUM are automatically added before the mapping procedure itself takes place. This mesh is only available when the two independent axis-variables have already been defined by the POLY command.</p>
	<p>SET_AXIS_VARIABLE</p> <p>For Y the POLY module always enforces the automatic procedures for adding initial equilibrium points during mapping. For N no initial equilibrium points are then added during mapping.</p>

## STOP\_ON\_ERROR

Useful for batch jobs in order to prevent that an erroneous sequence of commands to the program causes waste of computer activity.

Syntax	STOP_ON_ERROR
	<p>Give the preferred argument (ON or OFF) after the STOP command. If the default argument ON is given, the program terminates after an illegal or ambiguous command. It is possible to reset the effect of this command by giving the argument OFF.</p>



---

## TABULATION\_REACTION Commands

In this section:

---

<i>ENTER_FUNCTION</i> .....	246
<i>ENTER_REACTION</i> .....	247
<i>LIST_SUBSTANCES</i> .....	249
<i>SET_ENERGY_UNIT</i> .....	251
<i>SET_PLOT_FORMAT</i> .....	251
<i>SWITCH_DATABASE</i> .....	251
<i>TABULATE</i> .....	253
<i>TABULATE_DERIVATIVES</i> .....	253
<i>TABULATE_REACTION</i> .....	258
<i>TABULATE_SUBSTANCE</i> .....	260

## ENTER\_FUNCTION

Used to define a new thermodynamic function to be included in the sixth column of tabular output. The last entered function is listed in the 6th column of all tables, and can be plotted (if choosing the Plot Column value 6) in all graphs, for all subsequently tabulated substances or reactions.

Syntax	ENTER_FUNCTION
Prompt	NAME: <NAME> FUNCTION: <DEFINITION>
	A limited number of state variables, G, H, S, T, P, V and H298 can be used in the function definition. For example, $-(G-H)/T$ can be defined as a function which is identical to S for a substance or $\Delta S$ for a reaction, $G+T*S-P*V$ can be defined as a function which is U (internal energy) for a substance or $\Delta U$ (internal energy change) for a reaction.
Options	Name of the function (maximum 8 characters) and Definition of the function. A long function can be typed over several lines. A function should be terminated by a semicolon (;) or an empty line.

### Example Output

For the pure substance Fe (using the SSUB database), by entering a function as  $G+T*S-P*V$ , the following table is obtained by typing <Enter> in the prompt `Output file /SCREEN/:`, and the figure by typing 6 in the prompt `Plot column /2/:`

```
TAB: ENTER-FUNCTION
Name: InEnergy
Function: G+T*S-P*V;
TAB: TABULATE_SUBSTANCE
Substance (phase): Fe
Pressure /100000/: <Enter>
Low temperature limit /298.15/: <Enter>
High temperature limit /2000/: <Enter>
Step in temperature /100/: <Enter>
Output file /try1/: try2
Graphical output? /Y/: <Enter>
Plot column? /2/: 6
```

This gives the following output:

```
O U T P U T   F R O M   T H E R M O - C A L C
Column 6: InEnergy G+T*S-P*V
Phase : FE_S                      Pressure :      100000.00
```

Specie: FE

```

*****
      T      Cp      H      S      G      InEnergy
      (K)    (Joule/K)  (Joule)  (Joule/K)  (Joule)
*****
298.15  2.48446E+01  2.17972E-06  2.72800E+01  -8.13353E+03  2.17972E-06
300.00  2.48905E+01  4.60049E+01  2.74338E+01  -8.18414E+03  4.60049E+01
400.00  2.71299E+01  2.64957E+03  3.49085E+01  -1.13138E+04  2.64957E+03
500.00  2.93561E+01  5.47211E+03  4.11976E+01  -1.51267E+04  5.47211E+03
600.00  3.19293E+01  8.53245E+03  4.67701E+01  -1.95296E+04  8.53245E+03
700.00  3.50985E+01  1.18777E+04  5.19207E+01  -2.44667E+04  1.18777E+04
800.00  3.92042E+01  1.55830E+04  5.68623E+01  -2.99068E+04  1.55830E+04
900.00  4.49645E+01  1.97726E+04  6.17903E+01  -3.58387E+04  1.97726E+04
1000.00 5.42147E+01  2.46891E+04  6.69619E+01  -4.22728E+04  2.46891E+04
1100.00 4.55851E+01  2.99025E+04  7.19412E+01  -4.92328E+04  2.99025E+04 $ Stable
phase is FE_S2
1200.00 3.40840E+01  3.51037E+04  7.64466E+01  -5.66322E+04  3.51037E+04
1300.00 3.49398E+01  3.85549E+04  7.92086E+01  -6.44162E+04  3.85549E+04  1400.00
3.57994E+01  4.20918E+04  8.18293E+01  -7.24692E+04  4.20918E+04
1500.00 3.66636E+01  4.57149E+04  8.43287E+01  -8.07780E+04  4.57149E+04
1600.00 3.75330E+01  4.94247E+04  8.67226E+01  -8.93314E+04  4.94247E+04 $ Stable
phase is FE_S3
1700.00 4.05217E+01  5.41173E+04  8.95609E+01  -9.81363E+04  5.41173E+04
1800.00 4.12595E+01  5.82055E+04  9.18975E+01  -1.07210E+05  5.82055E+04 $ Stable
phase is FE_L
1900.00 4.60000E+01  7.74165E+04  1.02377E+02  -1.17099E+05  7.74165E+04  2000.00
4.60000E+01  8.20165E+04  1.04736E+02  -1.27456E+05  8.20165E+04

```

## ENTER\_REACTION

This is the same as [TABULATE\\_REACTION on page 258](#) in that both the chemical reaction can be specified and the thermodynamic property changes for the reaction can be generated as a table, and plotted as a graph or saved as an experimental file (with an extension of .EXP). The thermodynamic data are automatically retrieved from the SSUB5 database (by default), or the current database set by [SWITCH\\_DATABASE on page 20](#) (thus there is no need to use the DATA module before this command). You can select any other database by using the SWITCH\_DATABASE command in the TAB module. The rules to specify a reaction are the same as in the command TABULATE\_REACTION.

Syntax	ENTER_REACTION
Prompts	<p>SAME REACTION? /Y/: &lt;Y OR N&gt;</p> <p>This displays if there is at least one reaction already defined either by the command ENTER_REACTION or TABULATE_REACTION. For Y the next prompt for defining reaction is not asked.</p>
	<p>REACTION: &lt;CHEMICAL REACTION EQUATION&gt; &amp; &lt;RA+RB=PC+PD&gt;</p> <p>A long reaction can be typed over several lines. A reaction should be terminated by a semicolon (;) or an empty line. A list showing the used database, defined elements, getting-data sequence, references, etc.:</p> <p>Pressure /100000/: &lt;pressure of interest, in pa&gt;</p> <p>Low temperature limit /298.15/: &lt;T-low, in K&gt;</p> <p>High temperature limit /2000/: &lt;T-high, in K&gt; Step in temperature /100/: &lt;T-step&gt;</p>
	<p>OUTPUT FILE /SCREEN/: &lt;RETURN FOR SCREEN, OR TYPE A FILE NAME&gt;</p> <p>If you type Return for screen a list of thermodynamic property changes for the defined/chosen reaction is shown up as a table (which is demonstrated in the example outputs given below), and the command is terminated.</p> <p>If typing a file name, the table is displayed and saved as an *.EXP or an *.TAB file. Then prompts:</p>
	<p>GRAPHICAL OUTPUT /Y/: &lt;Y OR N&gt;</p> <p>For N a table is output to the screen and this table is saved as a basic text file with the default extension .TAB under the current working directory. In this case, the graph cannot be plotted.</p> <p>For Y a table is created with all thermodynamic functions as normal (which is displayed on screen) and generates a graph with temperature on the X-axis and a chosen property on a certain column in the table on the Y-axis (which is plotted on screen and saved as an *.EXP file), and it further asks which column is to be plotted on the resulting graph:</p>
	<p>PLOT COLUMN? /2/: &lt;1 OR 2 OR 3 OR 4 OR 5 OR 6&gt;</p> <p>Specify which property (as column number) to be plotted as the Y-axis (versus temperature as X-axis) as a graph on the screen. Simultaneously, all tabulated properties and the Y-axis setting (i.e. the plotted column) for the graph is written into an *.EXP file using the DATAPLOT format. The default column 2 is heat capacity, 3 enthalpy, 4 entropy and 5 Gibbs energy, and the additional column 6 is a user-entered function. The table displays on the screen. The plot then displays on the screen, followed by a POST prompt. The POST module (postprocessor) automatically opens, and all types of the POST-module commands to refine the plotted diagram may be used. Possibilities include scaling the</p>

Syntax	ENTER_REACTION
	X/Y-axis, changing the X/Y-axis texts, etc. The command BACK or EXIT at the POST prompt always takes you back to the TAB module.

## LIST\_SUBSTANCES

List all species in the current database with a certain set of elements. This is useful to specify species as pure substances in the command [TABULATE\\_SUBSTANCE](#) on page 260.

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

### Example Output

For the SSOL5 database, there are different lists, as shown below:

```
TAB: l-sub
With elements /*/: <Enter>
VA          AG          AL
AM          AS          AU
B           BA          BE BI  BR C
CA          CD          CE
CL          CO          CR
CS          CU          DY
ER          EU          F
FE          GA          GD
GE          H           HF
HG          HO          I
IN          IR          K
LA          LI          LU
MG          MN          MO
```

NA	NB	
ND	NI	NP
OS	P	
PA	PB	PD
PR	PT	PU
RB	RE	RH
RU	S	SB
SC	SE	SI
SM	SN	SR
TA	TB	TC
TE	TH	TI
TL	TM	U
V	W	Y
YB	ZN	ZR
C1	C2	C3
C4	C5	C6
C7	N2	O2
P1	P2	P4
NA/+1	K/+1	CL/-1
H2O	H1/+	LI1/+
CS1/+	RB1/+	O1H1/-
F1/-	BR1/-	I1/-
H1/+1	H1O1/-1	SI1O2 CA1O1 TAB:

TAB: l-sub

With elements /\*/: fe cr ni c n o

Exclusively with those elements? /Y/: <Enter>

C	CR	FE
N	NI	O
C	C2	C3
C	C5	C6
C	N2	O2

TAB:l-sub fe cr ni c n o

Exclusively with those elements? /Y/: n

C	CR	FE N	NI O
C1	C2	C3	
C4	C5	C6	

```
C7          N2          O2
H2O        O1H1/-      H1O1/-1 SI1O2 CA1O1 TAB:
```

## SET\_ENERGY\_UNIT

Set the energy unit as calories or Joule, in all the subsequent outputs (tables, graphs, and files) in the current calculation operation.

Syntax	SET_ENERGY_UNIT
Prompt	ENERGY UNIT (C=CAL, J=JOULE) /J/: <UNIT>

## SET\_PLOT\_FORMAT

Set the plotting format while the result is plotted on screen or the file is saved as EXP file [using DATAPLOT graphical format] and TAB file (as a basic text file and as displayed on screen).



This command is different from [SET\\_PLOT\\_FORMAT](#) on page 210 in the POST module, but is identical to [SET\\_PLOT\\_ENVIRONMENT](#) on page 243 in the SYS (system utility) monitor.

Syntax	SET_PLOT_FORMAT
Options	<p>The default set Unit is 1 (Windows) or 9 (Linux) for graphical presentation on screen, or all other units for outputs as *.EXP and *.TAB files.</p> <p>Also set the format of the graphical output to different graphical devices. The default unit 22 (1 for legacy Windows, and 9 for legacy Linux) may be altered with the SET_PLOT_ENVIRONMENT command in the SYS monitor or by the TC.INI file.</p>

## SWITCH\_DATABASE

By default, the TAB module always automatically retrieves thermodynamic data for substances or reactant/product substances in a defined reaction, or for pure phases or ideal solution phases, from the SSUB Substances Database. However, you can select thermodynamic data for complex non-ideal solution phases from another database. This is possible with this command.

This command switches (or changes) from the current database to a new one, and reinitializes the entire TAB module for defining a substance or reaction and the GIBBS workspace for storing retrieved data. All the directly connected databases as predefined by the original database initiation file (TC\_INITD.TDB file in the /DATA/ area for Windows environments, or the initd.tdb file in the \data\ area for Linux) are listed by pressing the <Enter> key without giving any argument. You can also supply your own database by giving the argument USER and then the database name and, if it is not located in the current working directory, its correct path.

This command (when required to use another database for subsequent tabulations) must be used before executing the TAB commands [TABULATE\\_SUBSTANCE](#) on page 260 for substances, and [ENTER\\_REACTION](#) on page 247 or [TABULATE\\_REACTION](#) on page 258 for reactions.

When a predefined database or an appropriate USER database is switched on, the DATA command [GET\\_DATA](#) on page 15 is automatically executed; therefore, the TAB module immediately displays a message

### Example

Example of TAB module message with the PSUB database specified

```
TAB: SW PSUB

THERMODYNAMIC DATABASE Module running on PC/Windows NT

Current database: TC Public Substances Database

VA DEFINED

REINITIATING GES5

VA DEFINED

ELEMENTS

SPECIES

PHASES


PARAMETERS

FUNCTIONS

-OK- TAB:
```

Syntax	SWITCH_DATABASE
Prompt	<p>DATABASE /XYZ/: &lt;NEW DATABASE NAME&gt;</p> <p>Specify a New database name. XYZ stands for the default SSUB database or the current database which is switched on. If an appropriate database name is not given and the USER option is not used, this list displays:</p> <p>Use one of these databases</p> <p>PURE4 = SGTE Pure Elements Database v4</p> <p>SSUB3 = SGTE Substances Database v3</p> <p>USER = user defined database</p> <p>DATABASE NAME /XYN/: &lt;new database name&gt;</p>
Notes	<p>DATABASE NAME: The new database is specified by typing the abbreviation given in the front of one of the available predefined databases. For convenience when switching/appending databases or recently purchased databases from Thermo-Calc Software or its agents, you can add them to the predefined database list in the database initiation file TC_INITD.TDB or initd.tdb of your installed software.</p>



Syntax	SWITCH_DATABASE
	<p>When this command is used in a MACRO (*.TCM) file, if the USER option is selected, the database setup file name (*setup.TDB) containing the setup definitions of the USER database, and its correct path, must be provided.</p> <p>If a USER database name or its path is not given on the same line of the SWITCH_DATABASE command, or if it is incomplete or incorrect, an Open window displays to specify the filename of the database setup file name (*setup.TDB) of the to-be-switched USER database.</p> <p> Unlike in the DATA module, if a USER database is used, the Gibbs energy system is also reinitialized and only data from the USER databases are retrieved for tabulations.</p> <p>After this command, those commands to define systems (in terms of either elements or species), to reject/restore phases or species, retrieve data, as well as to append data from additional database(s), can be done.</p>

## TABULATE

Gives the values of an already-defined table (with various properties varied with the stepping axis variable) from equilibria calculated with a STEP command. You can tabulate a table even if the table is entered after the STEP calculation.

Syntax	TABULATE
Prompts	<p>NAME: &lt;NAME OF A DEFINED TABLE&gt;</p> <p>The name of the table must be given. The table must be ENTERED.</p>
	<p>OUTPUT TO SCREEN OR FILE /SCREEN/: &lt;FILE NAME&gt;</p> <p>The table can be listed on the screen (by pressing &lt;Enter&gt;), on a file (the file name must be specified here).</p>

## TABULATE\_DERIVATIVES


This command is mainly for system debugging purposes and for experienced users. It automatically calculates all partial derivatives for a pure phase or solution phase at a given composition.



This is not the same as the chemical potential.

Before using this command, the system must be defined and thermodynamic data retrieved from an appropriate solution database in the DATA module. The phase name can be given in either upper, lower

or mixed cases, and can be abbreviated until it is unique, e.g. fcc, BCC, cem, Liq, etc. as the SSOL database is used for the tabulations, or GAS, FE-S, wustite, Fe2O3-hem, etc. as the SSUB database is used. The module then optionally goes through a specific sublattice or all the possible sublattices for the specified phase, as well as through the whole framework of a currently defined system (including all the defined elements/species, as well as the default defined vacancy and electron if necessary for the current database), when it prompts for inputs of site fractions for various species possibly occupying such sublattices. Therefore, thermodynamic properties can be tabulated for a pure phase, or for a solution phase as a pure end-member (with a composition definition for the corresponding non-interacting species on all necessary sublattices in the end-member), or for a solution phase as a real solution (with a composition definition for related interacting species on all necessary sublattices in the solution).

Syntax	TABULATE_DERIVATIVES
Prompts	<p>PHASE NAME /XXXX/: &lt;NAME OF THE PHASE&gt;</p> <p>Specify the phase name of a pure phase or a solution phase.</p> <p>XXXX is the last phase the TAB module accounted for. It automatically prompts for other options and necessary inputs for the definition of the composition of the specified phase.</p> <p>For a pure phase (such as Fe-S, Wustite, and Fe2O3-Hematite), no further composition definition is needed. For a solution phase with one sublattice (such as AQUEOUS solution, GAS mixture and SLAG solution), it requests <math>n-1</math> site-fraction inputs for the phase constituents (if there are <math>n</math> species in the defined phase within the whole framework of currently defined system, including all the defined elements/species, as well as the default defined vacancy and electron if necessary for the current database); the <math>n</math>th species is automatically assigned as the rest.</p> <div style="border: 1px solid black; background-color: #d4edda; padding: 10px; margin-top: 10px;">  The sum of input site fractions must not exceed unity. </div>
	<p><b>Example</b></p> <p>For example, these prompts and inputs can be seen for a LIQUID solution phase (from the SSOL database) within the Fe-Cr-Ni-C-N-O framework (Note that by default, the unprompted Ni species are assigned as the rest):</p> <pre> FRACTION OF CONSTITUENT (RETURN FOR PROMPT): &lt;RETURN&gt; C /1/: .05 CR /1/: .1 FE /1/: &lt; RETURN&gt; SUM OF FRACTIONS EXCEED UNITY, PLEASE REENTER FE /1/: .8 N /1/: .005 </pre> <p>For a solution phase with two or more sublattices (such as FCC alloy solution, and ION_</p>

Syntax	TABULATE_DERIVATIVES
	<p>LIQ ionic liquid solution), it first asks for which sublattice the site-fractions of constituents shall be specified: the default value 0 for all possible sublattices, and a given positive number for a specific sublattice (of course, this number must be reasonable for the currently specified phase, i.e. it must be smaller than the total sublattice number of the phase). Then, for the given sublattice or for all sublattices, it prompts for all the necessary inputs of site-fractions for the possible constituents on each sublattice n-1 times if there are n species on such a sublattice in the defined phase; the nth species on each of the sublattices is automatically assigned as the rest. For example, the following prompts and inputs can be seen for an FCC solution phase (from the SSOL5 database) within the Fe-Cr-Ni-C-N-O framework (Note that by default, the unprompted O species on its sublattice 1 and VA on its sublattice 2 are assigned as the rest):</p> <pre> SPECIFY SUBLATTICE (0 FOR ALL) /0/: &lt;RETURN&gt;  FRACTIONS IN SUBLATTICE 1  CR /1/: .1 FE /1/: .8 NI /1/: .0995  FRACTIONS IN SUBLATTICE 2  C /1/: .05 N /1/: .05 </pre>
	<pre>TEMPERATURE /2000/: &lt;TEMPERATURE OF INTEREST, IN K&gt;</pre> <p>Specify the temperature of interest in K.</p>
	<pre>PRESSURE /100000/: &lt;PRESSURE OF INTEREST, IN PA&gt;</pre> <p>Specify the pressure of interest in Pa.</p>

### Example Output

For the FCC phase in the Fe-Cr-Ni-C-N-O system (using the SSOL database), the following table is obtained at a specified composition:

```

TAB: TAB_DER

Phase name /BCC/: FCC

SPECIFY SUBLATTICE (0 FOR ALL) /0/: <Enter>

FRACTIONS IN SUBLATTICE 1

CR /1/: .1
FE /1/: .8
NI /1/: .3

SUM OF FRACTIONS EXCEED UNITY, PLEASE REENTER

```

---

```

NI /0/: .0995
FRACTIONS IN SUBLATTICE 2
C /1/: .05
N /1/: .05
Temperature /1800/: <Enter>
Pressure /100000/: <Enter>
Gibbs energy: ..... -1.27432533E+05
Helmholz energy: ..... -1.27433205E+05
Enthalpy: ..... 5.95773994E+04
Internal energy: ..... 5.95767279E+04
Entropy: ..... 1.03894407E+02
Molar volume: ..... 6.71473258E-06
Thermal expansivity: ..... 7.63886416E-05
Isothermal compressibility: ..... 6.02925387E-12
Heat capacity at constant pressure: 4.33555074E+01

First partial derivative with respect to CR in sublattice 1 of Gibbs energy:
..... -1.26034739E+05 of enthalpy: ..... 4.63000206E+04
of entropy: ..... 9.57415334E+01 of volume:
..... 6.87203263E-06

Second partial derivative of Gibbs energy with respect to also
CR in 1: 1.54392858E+05
FE in 1: -1.53353158E+04
NI in 1: -1.71750366E+04
O in 1: 0.00000000E+00
C in 2: -1.82016870E+05
in 2: -3.73062665E+05
VA in 2: -9.36260878E+04

First partial derivative with respect to FE in sublattice 1 of Gibbs energy:
..... -1.02869265E+05
of enthalpy: ..... 6.11738912E+04 of entropy:
..... 9.11350866E+01 of volume: .....
7.53441165E-06

Second partial derivative of Gibbs energy with respect to also
FE in 1: 1.82508696E+04
NI in 1: -3.07043434E+03
in 1: 0.00000000E+00
C in 2: -1.36027071E+05
in 2: -2.13007485E+05

```

---

---

VA in 2: -1.11741180E+05

First partial derivative with respect to NI in sublattice 1 of Gibbs energy:  
..... -1.32427029E+05 of enthalpy: ..... 5.21563580E+04  
of entropy: ..... 1.02546326E+02 of volume:  
..... 0.00000000E+00

Second partial derivative of Gibbs energy with respect to also

NI in 1: 1.48390257E+05

in 1: 0.00000000E+00

C in 2: -7.70620431E+04

in 2: -1.61551726E+05

VA in 2: -1.12772206E+05

First partial derivative with respect to O in sublattice 1 of Gibbs energy:  
..... -2.62929308E+05 of enthalpy: ..... 5.02555370E+04  
of entropy: ..... 1.73991581E+02 of volume:  
..... 0.00000000E+00

Second partial derivative of Gibbs energy with respect to also

in 1: 2.99322360E+07

C in 2: 0.00000000E+00

N in 2: 0.00000000E+00

VA in 2: -1.82377137E+05

First partial derivative with respect to C in sublattice 2 of Gibbs energy:  
..... -1.59508417E+05 of enthalpy: ..... 1.21269096E+05  
of entropy: ..... 1.55987507E+02 of volume:  
..... 1.06885187E-05

Second partial derivative of Gibbs energy with respect to also

C in 2: 2.99322360E+05

N in 2: -1.90144000E+04

VA in 2: -2.78465070E+04

First partial derivative with respect to N in sublattice 2 of Gibbs energy:  
..... -2.39671400E+05 of enthalpy: ..... 4.04456947E+04  
of entropy: ..... 1.55620608E+02 of volume:  
..... 0.00000000E+00

Second partial derivative of Gibbs energy with respect to also

N in 2: 2.99322360E+05

VA in 2: -3.30383665E+04

First partial derivative with respect to VA in sublattice 2 of Gibbs energy:  
..... -9.52042686E+04 of enthalpy: ..... 5.37142294E+04  
of entropy: ..... 8.27324989E+01 of volume:  
..... 6.86700739E-06

Second partial derivative of Gibbs energy with respect to also

VA in 2: 1.66290200E+04

---

## TABULATE\_REACTION


Tabulate thermodynamic property changes for a chemical reaction as a table, or variation of one chosen property can be plotted against temperature as a graph, or saved as an experimental file (with an extension of .EXP). The thermodynamic data are automatically retrieved from the SSUB5 database (by default), or the current database set by the SWITCH\_DATABASE command (thus there is no need to use the DATA module before this command). You can select any other database by using [SWITCH\\_DATABASE on page 251](#) in the TAB module.

It is important to remember the rules to specify a reaction:

- The reaction is specified, by giving the reactants and products, such as  $\text{Ga} + \text{S} = \text{GaS}$ ,  $5\text{Al} + 2\text{Fe} = \text{Al}_5\text{Fe}_2$ .
- Under Linux environments, the notation for a chemical formula treats upper and lower cases as the same (such as  $\text{ga} + \text{s} = \text{GaS}$ ,  $5\text{Al} + 2\text{Fe} = \text{al}_5\text{fe}_2$ ); but under Windows, the TAB module only accepts upper cases, e.g.  $\text{GA} + \text{S} = \text{GAS}$ ,  $5\text{AL} + 2\text{FE} = \text{AL}_5\text{FE}_2$ .
- Elements with a single letter symbol must be followed by a stoichiometry factor, even if it is 1; thus, the symbol  $\text{CO}$  is taken as cobalt, carbon monoxide must be given as  $\text{C1O1}$  (or  $\text{O1C1}$ ).
- All the reactants and products must be defined as species-stoichiometries in the currently-used database; in other words, the reaction definition only accepts already-defined species-stoichiometries as reactants and products. For example, if a database does not have a species defined with a stoichiometry of  $\text{Al}_5\text{Fe}_2$  {e.g. the Al and Fe (but not  $\text{Al}_5\text{Fe}_2$ ) may be defined as species, and the  $\text{Al}_5\text{Fe}_2$  phase may be defined as a two-sublattice stoichiometric phase  $[\text{Al}]_5[\text{Fe}]_2$ , rather than a single sublattice stoichiometric phase  $[\text{Al}_5\text{Fe}_2]$ }, then the reaction  $5\text{Al} + 2\text{Fe} = \text{Al}_5\text{Fe}_2$  cannot be tabulated.
- Make sure that the Gibbs free energy expression for a stoichiometric phase is really corresponding to the species-stoichiometry. For example, if a database has a definition of Function  $\text{GAL}_5\text{FE}_2$  for 1/7 of the  $\text{AL}_5\text{FE}_2$  formula, then the relation  $\text{G}(\text{Al}_5\text{Fe}_2) = 7 * \text{GAL}_5\text{FE}_2$  must be defined; otherwise, the tabulated thermodynamic properties for the reaction  $5\text{Al} + 2\text{Fe} = \text{Al}_5\text{Fe}_2$  is wrong.

Syntax	TABULATE_REACTION
Prompts	<p>SAME REACTION? /Y/: &lt;Y OR N&gt;</p> <p>This prompt displays if there is at least one reaction already defined either with the commands <a href="#">ENTER_REACTION on page 247</a> or TABULATE_REACTION. If you answer Y, then the next prompt is not asked.</p> <p>REACTION: &lt;CHEMICAL REACTION EQUATION&gt; &amp; &lt;RA+RB=PC+PD&gt;</p> <p>A long reaction can be typed over several lines. A reaction should be terminated by a</p>

Syntax	TABULATE_REACTION
	<p>semicolon (;) or an empty line. A list showing the used database, defined elements, getting-data sequence, references, etc.</p> <pre>Pressure /100000/: &lt;pressure of interest, in pa&gt;</pre> <p>Low temperature limit /298.15/: &lt;T-low, in K&gt; Specify the starting temperature K.</p> <p>High temperature limit /298.15/: &lt;T-high, in K&gt; Specify the ending temperature K. Step in temperature /100/: &lt;T-step&gt; Specify the temperature step for the tabulation.</p>
	<pre>OUTPUT FILE /SCREEN/: &lt;RETURN FOR SCREEN, OR TYPE A FILE NAME&gt;</pre> <p>If you type Return for screen, a list of thermodynamic property changes for the defined/chosen reaction is shown as a table (which is demonstrated in the example outputs given below), and the command is terminated.</p> <p>If typing a file name, the table is both displayed on screen and saved as an *.EXP or a *.TAB file, and the program prompts:</p>
	<pre>GRAPHICAL OUTPUT /Y/: &lt;Y OR N&gt;</pre> <ul style="list-style-type: none"> <li>• For N a table is output to the screen, and the same table is saved as a basic text file with the default extension .TAB under the current working directory. In this case, the graph cannot be plotted.</li> <li>• For Y a table is created with all thermodynamic functions as normal (which is displayed on screen) and generates a graph with temperature on the X-axis and a chosen property on a certain column in the table on the Y-axis (which is plotted on screen and saved as an *.EXP file), and it also asks which column is to be plotted on the resulting graph:</li> </ul>
	<pre>PLOT COLUMN? /2/: &lt;1 OR 2 OR 3 OR 4 OR 5 OR 6&gt;</pre> <p>Specify which property (as column number) to be plotted as the Y-axis (versus temperature as X-axis) as a graph on the screen. Simultaneously, all tabulated properties and the Y-axis setting (i.e. the plotted column) for the graph is written into an *.EXP file using the DATAPLOT format. The default column 2 is heat capacity, 3 enthalpy, 4 entropy and 5 Gibbs energy, and the additional column 6 is a user-entered function. The table displays on the screen. The plot then displays on the screen, followed by a POST: prompt. The POST module (postprocessor) automatically opens, and all types of the POST-module commands to refine the plotted diagram may be used. Possibilities include scaling the X/Y-axis, changing the X/Y-axis texts, etc. The command BACK or EXIT at the POST: prompt always takes you back to the TAB module.</p>

Syntax	TABULATE_REACTION
	 Also see the <i>DATPLOT User Guide</i> included with this documentation set.

## Example Output

For the reaction  $\text{Ga} + \text{S} = \text{GaS}$  (using the SSUB5 database), the following table is obtained by typing <Enter> in the prompt Output file /SCREEN/, and the figure by typing 2 in the prompt Plot column /2/:

```

O U T P U T   F R O M   T H E R M O - C A L C

Reaction:  S+GA=GA1S1

stable as S_S
GA stable as GA_S
GA1S1 stable as GA1S1_S

Delta-Cp      Delta-H      Delta-S      Delta-G
(K)      (Joule/K)      (Joule)      (Joule/K)      (Joule)
*****
298.15  -2.79489E+00  -2.09200E+05  -1.50580E+01  -2.04710E+05
300.00  -2.87516E+00  -2.09205E+05  -1.50755E+01  -2.04683E+05
302.    ---- GA becomes GA_L ,delta-H =    5589.80
367.    ---- S becomes S_S2 ,delta-H =    401.00
389.    ---- S becomes S_L ,delta-H =    1721.00
400.00  -1.22278E+01  -2.17521E+05  -4.07488E+01  -2.01222E+05
500.00  -1.57686E+01  -2.19323E+05  -4.47280E+01  -1.96959E+05
600.00  -1.02518E+01  -2.20583E+05  -4.70410E+01  -1.92359E+05
700.00  -6.58954E+00  -2.21430E+05  -4.83534E+01  -1.87583E+05
800.00  -4.46246E+00  -2.21963E+05  -4.90686E+01  -1.82709E+05
900.00  -2.82671E+00  -2.22328E+05  -4.94995E+01  -1.77778E+05
1000.00 -1.21787E+00  -2.22530E+05  -4.97138E+01  -1.72816E+05
1100.00  3.71702E-01  -2.22572E+05  -4.97552E+01  -1.67841E+05

```

## TABULATE\_SUBSTANCE



Tabulate thermodynamic properties of a substance (with a given chemical formula but it is not certain in which phase/state it may form) or a pure stoichiometric phase (getting data from a specific substance database such as SSUB5, or from a specific solution database such as SSOL5 and TCFE8), or of a solution phase with a fixed composition (getting data from a specific solution database such as SSOL5 and TCFE8), under a constant pressure and various temperatures.



---


In case of a pure stoichiometric phase or a solution phase with a fixed composition, you must already define the system and get thermodynamic data from an appropriate solution database in the DATA module before using this TAB command. The phase name can be given either upper or lower or mixed cases, and can be abbreviated until it is unique, e.g. *fcc*, *BCC*, *Liq*, *cem*, *Al<sub>5</sub>Fe<sub>2</sub>*, etc. as the SSOL database is used for the tabulations, or *GAS*, *FE-S*, *wustite*, *Fe<sub>2</sub>O<sub>3</sub>-hem*, etc. as the SSUB database is used. The module then optionally goes through a specific sublattice or all the possible sublattices for the specified phase, as well as through the whole framework of a currently defined system (including all the defined elements/species, as well as the default defined vacancy and electron if necessary for the current database), when it prompts for inputs of site fractions for various species possibly occupying such sublattices. Therefore, you can tabulate thermodynamic properties for a pure phase, or for a solution phase as a pure end-member (with a composition definition for the corresponding non-interacting species on all necessary sublattices in the end-member), or for a solution phase as a real solution (with a composition definition for related interacting species on all necessary sublattices in the solution).

Moreover, the variation for one of the tabulated properties for a substance, a pure stoichiometric phase, or a solution phase with a fixed composition can be plotted against temperature as a graph or saved as an experimental file (with an extension of .EXP).

Syntax	<b>TABULATE_SUBSTANCE</b>
Prompt	<p>SUBSTANCE (PHASE) : &lt;NAME OF THE SPECIES OR PHASE&gt;</p> <p>In case of a substance, give its chemical formula, e.g. Fe, H<sub>2</sub>, C<sub>1</sub>H<sub>6</sub>, FeC<sub>1</sub>, CaC<sub>1</sub>O<sub>3</sub>, MgSiO<sub>3</sub>, etc. When the TABULATE_SUBSTANCE &lt;SUBSTANCE&gt; command sequence is used for the first time in the TAB module, it always uses the SSUB Substances Database as the default database. If the SSUB database is not available for the current Thermo-Calc installation and a specific database has not been switched on yet, it may prompt to specify an appropriate substance or solution database (e.g. typing SSUB2, SSUB3, SSUB4, SSUB5; SSOL2, SSOL4, SSOL5; TCFE3, TCFE4, TCFE5, TCFE6, TCFE7, TCFE8 etc.). Prior to this command, you can also use the <a href="#">SWITCH_DATABASE on page 251</a> command in the TAB module to set the current database. If a solution database is set as the current database, only the neutral species that are valid substance standing by themselves as phases can be tabulated.</p> <p> Before other prompts, a list of the used database, defined elements, getting-data sequence, references, etc. is displayed on screen. From such information, you know what the TAB module is performing.</p> <p>In case of a pure stoichiometric phase or a solution phase, give its phase name, e.g. FCC, CEMENTITE, LIQUID, SLAG, AQUEOUS, GAS, Al<sub>5</sub>Fe<sub>2</sub>, Fe-S, Wustite, Fe<sub>2</sub>O<sub>3</sub>-Hematite, etc.</p> <div style="border: 1px solid black; background-color: #d4edda; padding: 10px; margin: 10px 0;"> <p> <b>REMEMBER:</b> It is important that you have already defined the system and gotten thermodynamic data from an appropriate solution database in the DATA module before using this TAB_SUB command. It automatically prompts for other options and necessary inputs for the definition of the composition of the specified phase.</p> </div> <p>For a pure stoichiometric phase defined with one single sublattice (such as Fe-S, Wustite, and Fe<sub>2</sub>O<sub>3</sub>-Hematite), no further composition definition is needed.</p> <p>For a solution phase defined with one sublattice (such as AQUEOUS solution, GAS mixture and SLAG solution), it requests <math>n-1</math> site-fraction inputs for the phase constituents (if there are <math>n</math> species in the defined phase within the whole framework of currently defined system, including all the defined elements/species, as well as the default defined vacancy and electron if necessary for the current database); the <math>n</math>th species is automatically assigned as the rest.</p>

Syntax	TABULATE_SUBSTANCE
	<div>  <p>The sum of input site fractions must not exceed unity. For example, the following prompts and inputs can be seen for a LIQUID solution phase (from the SSOL database) within the Fe-Cr-Ni-C-N-O framework (Note that by default, the unprompted Ni species is assigned as the rest):</p> </div>
	<pre> FRACTION OF CONSTITUENT (RETURN FOR PROMPT) : &lt;RETURN&gt;  C /1/: .05  CR /1/: .1  FE /1/: &lt;RETURN&gt; </pre>
	<pre> SUM OF FRACTIONS EXCEED UNITY, PLEASE REENTER  FE /1/: .8  N /1/: .005 </pre> <p>For a pure stoichiometric phase defined with two or more sublattices (such as Al<sub>5</sub>Fe<sub>2</sub> inter-metallic stoichiometric phase) and for a solution phase defined with two or more sublattices (such as FCC alloy solution, and ION_LIQ ionic liquid solution, Al<sub>5</sub>Fe<sub>4</sub> inter-metallic solution phase), it first asks for which sublattice the site-fractions of constituents shall be specified: the default value 0 for all possible sublattices, and a given positive number for a specific sublattice (this number must be reasonable for the currently specified phase, i.e. it must be smaller than the total sublattice number of the phase). Then, for the given sublattice or for all sublattices, it prompts for all the necessary inputs of site-fractions for the possible constituents on each sublattice <math>n-1</math> times if there are <math>n</math> species on such a sublattice in the defined phase; the <math>n</math>th species on each of the sublattices are automatically assigned as the rest. For example, these prompts and inputs can be seen for an FCC solution phase (from the SSOL database) within the Fe-Cr-Ni-C-N-O framework (Note that by default, the unprompted O species on its sublattice 1 and VA on its sublattice 2 is assigned as the rest):</p>
	<pre> SPECIFY SUBLATTICE (0 FOR ALL) /0/: &lt;RETURN&gt;  FRACTIONS IN SUBLATTICE          1  CR /1/: .1  FE /1/: .8  NI /1/: .0995  FRACTIONS IN SUBLATTICE          2  C /1/: .05  N /1/: .05 </pre>

Syntax	TABULATE_SUBSTANCE
	<p>PRESSURE /100000/: &lt;PRESSURE OF INTEREST, IN PA&gt;</p> <p>Specify the constant pressure condition in Pa.</p>
	<p>LOW TEMPERATURE LIMIT /298.15/: &lt;T-LOW, IN K&gt;</p> <p>Specify the starting temperature K.</p>
	<p>HIGH TEMPERATURE LIMIT /298.15/: &lt;T-HIGH, IN K&gt;</p> <p>Specify the ending temperature K.</p>
	<p>STEP IN TEMPERATURE /100/: &lt;T-STEP&gt; SPECIFY THE TEMPERATURE STEP FOR THE TABULATION.</p>
	<p>OUTPUT FILE /SCREEN/: &lt;RETURN FOR SCREEN, OR TYPE A FILE NAME&gt;</p> <p>If you type <code>Return for screen</code> a list of basic thermodynamic functions for the chosen substance or for the specified pure or solution phase with the fixed composition is shown up as a table (which is demonstrated in the example outputs given below), and the command is terminated.</p> <p>If typing a file name, the table is both displayed on screen and saved as an *.EXP or a *.TAB file, and the program further prompts:</p>
	<p>GRAPHICAL OUTPUT /Y/: &lt;Y OR N&gt;</p> <ul style="list-style-type: none"> <li>• For <code>N</code> a table is output to the screen, and the same table is saved as a basic text file with the default extension .TAB under the current working directory. In this case, the graph cannot be plotted.</li> <li>• For <code>Y</code> a table is created with all the thermodynamic functions as normal (which is displayed on screen) as well as generates a graph with temperature on the X-axis and a chosen property on a certain column in the table on the Y-axis (which is plotted on screen and saved as an *.EXP file), and it also ask which column is to be plotted on the resulting graph:</li> </ul>
	<p>PLOT COLUMN ? /2/: &lt;1 OR 2 OR 3 OR 4 OR 5 OR 6&gt;</p> <p>Specify which property (as column number) to be plotted as the Y-axis (versus temperature as X-axis) as a graph on the screen. Simultaneously, all tabulated properties and the Y-axis setting (i.e. the plotted column) for the graph is written into an *.EXP file using the DATAPLOT format. The default column 2 is heat capacity, 3 enthalpy, 4 entropy and 5 Gibbs energy, and the additional column 6 is a user-entered function. The table displays on the screen. The plot then displays on the screen, followed by a POST: prompt. The POST module (postprocessor) automatically opens, and all types of the POST-module commands to refine the plotted diagram may be used. Possibilities include scaling the X/Y-</p>

Syntax	TABULATE_SUBSTANCE
	axis, changing the X/Y-axis texts, etc. The command BACK or EXIT at the POST: prompt always takes you back to the TAB module.
	 Also see the <i>DATPLOT User Guide</i> included with this documentation set.

### Example Output 1

For the FCC alloy phase as a non-ideal solution with a fixed composition

[Fe0.80,Cr0.10,Ni0.0995,O0.005][C0.05,N0.05,VA0.90]

The following table is obtained by typing Return for screen at the prompt Output file /SCREEN/:

```

O U T P U T   F R O M   T H E R M O - C A L C

Phase : FCC                                Pressure :      100000.00
Specie: CR1/--2

*****
      T           Cp           H           S           G
      (K)        (Joule/K)    (Joule)    (Joule/K)    (Joule)
*****
298.15  2.70517E+01  6.23824E+03  4.40241E+01 -6.88755E+03
300.00  2.70889E+01  6.28832E+03  4.41916E+01 -6.96915E+03
400.00  2.87304E+01  9.08420E+03  5.22235E+01 -1.18052E+04
500.00  2.99904E+01  1.20222E+04  5.87742E+01 -1.73649E+04
600.00  3.10889E+01  1.50770E+04  6.43408E+01 -2.35275E+04
700.00  3.21116E+01  1.82375E+04  6.92106E+01 -3.02100E+04
800.00  3.30994E+01  2.14982E+04  7.35633E+01 -3.73524E+04
900.00  3.40742E+01  2.48569E+04  7.75182E+01 -4.49094E+04
1000.00 3.50483E+01  2.83130E+04  8.11586E+01 -5.28456E+04
1100.00 3.60268E+01  3.18667E+04  8.45449E+01 -6.11327E+04
1200.00 3.70143E+01  3.55187E+04  8.77219E+01 -6.97476E+04
1300.00 3.80149E+01  3.92700E+04  9.07241E+01 -7.86713E+04
1400.00 3.90311E+01  4.31222E+04  9.35784E+01 -8.78875E+04
1500.00 4.00649E+01  4.70768E+04  9.63064E+01 -9.73827E+04
1600.00 4.11174E+01  5.11358E+04  9.89256E+01 -1.07145E+05
1700.00 4.21896E+01  5.53010E+04  1.01450E+02 -1.17165E+05
1800.00 4.33555E+01  5.95774E+04  1.03894E+02 -1.27433E+05

```

1900.00	4.58528E+01	6.40379E+04	1.06306E+02	-1.37943E+05
2000.00	4.75402E+01	6.87138E+04	1.08704E+02	-1.48694E+05

## Example Output 2



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

For the H2 species as a pure substance (using the SSUB5 database), the following table is obtained by typing Return for screen at the prompt Output file /SCREEN/, whilst the figure is generated by typing 5 at the prompt Plot column /2/:

```

      O U T P U T F R O M T H E R M O - C A L C
Phase : GAS                      Pressure :      100000.00
Specie: H2
*****
H          S          G          T          Cp
(K)      (Joule/K)    (Joule)    (Joule/K)    (Joule)
*****
3.17684E-06  1.30680E+02 -3.89622E+04  298.15  2.88369E+01
300.00  2.88473E+01  5.33580E+01  1.30858E+02 -3.92042E+04
400.00  2.91591E+01  2.95686E+03  1.39209E+02 -5.27268E+04
500.00  2.92650E+01  5.87874E+03  1.45729E+02 -6.69856E+04
600.00  2.93441E+01  8.80908E+03  1.51071E+02 -8.18336E+04
700.00  2.94579E+01  1.17488E+04  1.55602E+02 -9.71730E+04
800.00  2.96320E+01  1.47027E+04  1.59547E+02 -1.12935E+05
900.00  2.98786E+01  1.76776E+04  1.63050E+02 -1.29068E+05
1000.00  3.02043E+01  2.06810E+04  1.66214E+02 -1.45533E+05
1100.00  3.05319E+01  2.37171E+04  1.69108E+02 -1.62302E+05
1200.00  3.09281E+01  2.67897E+04  1.71781E+02 -1.79348E+05
1300.00  3.13615E+01  2.99040E+04  1.74274E+02 -1.96652E+05
1400.00  3.18115E+01  3.30625E+04  1.76614E+02 -2.14197E+05
1500.00  3.22641E+01  3.62664E+04  1.78824E+02 -2.31970E+05
1600.00  3.27094E+01  3.95151E+04  1.80921E+02 -2.49958E+05
1700.00  3.31406E+01  4.28078E+04  1.82917E+02 -2.68151E+05
1800.00  3.35526E+01  4.61426E+04  1.84823E+02 -2.86539E+05
1900.00  3.39415E+01  4.95175E+04  1.86648E+02 -3.05113E+05
2000.00  3.43045E+01  5.29300E+04  1.88398E+02 -3.23866E+05

```

---

## TERNARY\_DIAGRAM Commands

In this section:

---

<i>TERNARY_DIAGRAM Module</i> .....	<i>268</i>
-------------------------------------	------------

## TERNARY\_DIAGRAM Module

The TERNARY\_DIAGRAM module (short name, the TERN module) enables you to quickly calculate a simple ternary phase diagram.

To enter the module, at the SYS prompt type GOTO\_MODULE TERNARY. There are no other commands for this module. Follow the prompts to plot a diagram.



Also see the Graphical Mode equivalent to this command, [Ternary Calculator](#) on page 106 as described in the *Thermo-Calc User Guide*.

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



---

## Thermodynamic Variables and Units

The following topics are about the different thermodynamic variables recognised by Thermo-Calc. The topics have information about how to define new derived variables and functions and how to express thermodynamic variables in non-default units. The POLY module only recognises default units, which are the SI units.



See example 44 [Thermo-Calc Console Mode Examples](#) to learn about using variables and functions.

In this section:

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<i>Thermodynamic Variables</i> .....	<a href="#">270</a>
<i>Derived Variables and Partial Derivatives</i> .....	<a href="#">281</a>
<i>Units of State Variables and Derived Variables</i> .....	<a href="#">288</a>

## Thermodynamic Variables

There are different thermodynamic variables in Thermo-Calc. Some are *state variables* such as temperature, pressure and mole fraction. These characterize the equilibrium state of a system. You set them when you define your system in the POLY module before performing a calculation. They are also used in other modules such as DATA, GIBBS and PARROT. State variables that involve components can be used for the defined components, but not for any species. (To define new components in a defined system, use [DEFINE\\_COMPONENTS](#) on page 143).

Other useful thermodynamic variables are derived from state variables with a mathematical function. Some derived variables are pre-defined by Thermo-Calc, such as normalized energetic and compositional extensive state variables for example. You use these by appending various normalizing suffixes to abbreviations that are associated with the state variables.

Thermodynamic variables can also be divided into extensive variables and intensive variables. An extensive variable is a variable whose value depends on the size of the system, whereas an intensive variable is a variable whose value is independent of system size.

More information about thermodynamic variables is available in the online help in Thermo-Calc Console Mode. Use the command [INFORMATION](#) on page 5, with a subject keyword such as one of the following as argument: STATE VARIABLES, INTENSIVE VARIABLES, EXTENSIVE VARIABLES, DERIVED VARIABLES, CONDITIONS (for condition settings), AXIS-VARIABLES (for stepping/mapping variable settings).

### Common Thermodynamic Variables

The tables below list common thermodynamic variables. Most of these can be used to define equilibrium conditions in the POLY module unless otherwise indicated.

The variables are divided into the following tables:

- Intensive variables
- Energy-related extensive variables for whole system or for a phase
- Compositional extensive variables (overall amount/size of components in whole system, or amount of a component in system or in a phase)
- Constitutional composition-related extensive variables (amount of a constituent/species on a sublattice site in a phase)
- Special quantities

#### *How to Read the Tables*

- The *Abbrev.* column shows the abbreviation that you use in the POLY module for referring to the variable. If the variable must be given any arguments, then these are given in parenthesis directly after the abbreviation. For most variables, this is also the abbreviation that you use to refer to the variable in other modules. However, some variables

are referred to with a different abbreviation in the POST module. If this is the case, then this is noted at the bottom of the table.

- Variables that are specific to a species, in which case the species is specified as an argument (*sp* in the table below). If there are two or more sublattices in a given phase, then this argument is given as `constituent#sublattice`. This indicates a constituent on a specific sublattice or site in the phase (referred to by the # sign and a digit). For example, `y(BCC,C#2)` stands for the site fraction of the C species on the second sublattice site of the BCC\_A2 solution phase.
- The *Unit* column show which unit that you can use to express the variable in the POLY module. This unit is always the SI unit. In other modules, state variables may be expressed in other units.
- The *Suffix* column shows the suffixes you can append to the variables. The R-suffix can be used with all compositional extensive state variables, but the suffix does not change the value of the variable. This is indicated by putting the R in parenthesis.

These types of variables are listed in the following topics:

- [Intensive Variables below](#)
- [Extensive Variables on the next page](#)
- [Special Quantities on page 275](#)
- [The u-Fraction Variable on page 276](#)
- [Suffixes on page 276](#)

## Intensive Variables

V	Abbrev.	Unit	Descript.	Domain	Suffix
T	T <sup>1</sup>	K	Temperature	System	
P	P	Pa	Pressure	System	
μ	MU(comp)	J/mol	Chemical potential	Component	R
	MU(sp,ph) <sup>2</sup>			Species relative to a solution phase	R

V	Abbrev.	Unit	Descript.	Domain	Suffix
a	AC(comp)	N/A	Activity	Component	R
	AC(sp,ph) <sup>2</sup>			Species relative to a solution phase	R
	LNAC (comp) <sup>3</sup>		ln(Activity)	Component	R
	LNAC (sp,ph) <sup>2</sup>			Species relative to a solution phase	R

<sup>1</sup> When plotting in POST, besides T (Kelvin), you can also use T\_C or T\_F to plot temperature in °C or °F.

<sup>2</sup> Only for single-substitutional-lattice solution phases such as AQUEOUS solution and GASEous mixture phases and for interacting species on the substitutional sublattice of two-sublattice solution phases (such as the phases BCC\_A2 and M6C phases).

<sup>3</sup> ln natural logarithm (lnAC=MU/RT)

## Extensive Variables

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



See example 44 in the *Console Mode Examples Guide* for an example of using variables and functions.

V	Abbrev.	Unit	Descript.	Domain	Suffix
V	V	m3	Volume	System	M, W, V, R
	V(ph) <sup>1</sup>			Phase	M, W, F, R
	VP(ph) <sup>2</sup>			Phase	M, W, V, R
G	G	J	Gibbs energy	System	M, W, V, R
	G(ph) <sup>1</sup>			Phase	M, W, V, F, R
A	A	J	Helmholtz energy	System	M, W, V, R
	A(ph) <sup>1</sup>			Phase	M, W, V, F, R

V	Abbrev.	Unit	Descript.	Domain	Suffix
U	U	J	Internal energy	System	M, W, V, R
	U(ph) <sup>1</sup>			Phase	M, W, V, F, R
H	H	J	Enthalpy	System	M, W, V, R
	H(ph)			Phase	M, W, V, F
S	S	J/K	Entropy	System	M, W, V, R
	S(ph) <sup>1</sup>			Phase	M, W, V, F, R
Cp	HM.T <sup>3</sup>	J/mol/K	Heat capacity at constant pressure	System	R
	HM(ph).T <sup>3</sup>			Phase	R
Cv	HM.T <sup>4</sup>	J/mol/K	Heat capacity at constant volume	System	R
	HM(ph).T <sup>4</sup>			Phase	R
D	DG(ph) <sup>5</sup>	N/A	Driving force (thermodynamic factor)	Phase	Always use with M, W, V or F. R can also be used.

<sup>1</sup> For this variable, if the phase is unstable, then the variable gets a value of zero.

<sup>2</sup> Do not use VP(ph) as a condition in POLY. Instead, use CHANGE\_STATUS PHASE <PHASE>=FIX <AMOUNT> where the fixed <AMOUNT> is roughly equal to VPF(ph), which cannot be directly evaluated or listed. If the phase is unstable, then VP(ph) and its normalized quantities get zero value.

<sup>3</sup> Use only if pressure has been set as a condition.

<sup>4</sup> Use only if volume has been set as a condition.

<sup>5</sup> Already divided by RT.

## Compositional Extensive Variables

These are for the overall amount/size of components in whole system, or amount of a component in system or in a phase.

For NP(ph) or BP(ph), these cannot be used in the POLY module. Instead use CHANGE\_STATUS PHASE <PHASE>=FIX <AMOUNT> where the fixed <AMOUNT> is roughly equal to NPF(ph) or BPF(ph), which cannot be directly evaluated or listed. If the phase is unstable, then NP(ph) or BP(ph) (and its normalized quantities) get zero value.

When plotting the following quantities in POST, refer to each as indicated:

- $X(\text{comp})$  > Mole-Fraction <comp> (or  $M_F$ )
- $W(\text{comp})$  > Weight-Fraction <comp> (or  $W_F$ )
- $X\%(\text{comp})$  > Mole-Percent <comp> (or  $M_P$ )
- $W\%(\text{comp})$  > Weight-Percent <comp> (or  $W_P$ ).
- $u-f(\text{ph}, \text{comp})$  > U-F

V	Abbrev.	Unit	Descript.	Domain	Suffix	Comment
n	N	mole	Moles	All components	M, W, V, (R)	
	N(comp)			Component	M, W, V, (R)	
	N(ph,comp)			Component in a phase	M, W, V, (R)	
	NP(ph) <sup>1</sup>			Phase	M, W, V, (R)	See above
b	B	gram	Mass	All components	M, W, V, (R)	
	B(comp)			Component	M, W, V, (R)	
	B(ph,comp)			Component in a phase	M, W, V, (R)	
	BP(ph) <sup>1</sup>			Phase	M, W, V, (R)	See above
x	X(comp)	N/A	Mole fraction	Component	(R)	See above
	X(ph,comp)			Component in a phase	(R)	
w	W(comp)	N/A	Mass (weight) fraction	Component	(R)	See above
	W(ph,comp)			Component in a phase	(R)	
x%	X%(comp) <sup>2</sup>	N/A	Mole percent	Component	(R)	See above
w%	W%(comp) <sup>2</sup>	N/A	Mass (weight) percent	Component	(R)	See above
u	u-f (ph,comp) <sup>1</sup>	N/A	u-fraction	Component in a stable phase	(R)	See above

V	Abbrev.	Unit	Descript.	Domain	Suffix	Comment
in	IN(sp) <sup>2</sup>	mole	Input mole number	Phase species in the system	(R)	See above
im	IM(sp) <sup>2</sup>	gram	Input mass unit	Phase species in the system	(R)	See above
<sup>1</sup> Do not use in the POLY module.						
<sup>2</sup> Only available in TQ-Interface and TC-API.						

### Constitutional Composition-Related Extensive Variable

This is the amount of a constituent/species on a sublattice site in a phase.

V	Abbrev.	Unit	Descript.	Domain
y	Y (ph,cons#sub)	N/A	Site fraction	Constituent on a sublattice site (denoted by # and a digit) in a phase

### Special Quantities

V	Abbrev.	Unit	Descript.	Domain	Suffix
Q	QF(ph) <sup>1</sup>	N/A	Phase stability function	Phase	R Under a condition and system definition, QFR (ph) = QF(ph)
Tc	TC(ph) <sup>2</sup>	K	Curie temperature	Phase	R Under a condition and system definition, TCR (ph) = TC(ph)
Mb	BMAG(ph) <sup>3</sup>	N/A	Bohr magneton number	Phase	R Under a condition and system definition, BMAGR (ph) = BMAG(ph)
<sup>1</sup> Negative when phase composition is inside a spinodal, otherwise positive. Can be used to find out if an equilibrium is within the miscibility gap for a solution phase. Cannot be used as a condition.					
<sup>2</sup> Calculated for phases with magnetic contributions in an equilibrium state. Cannot be used as a condition, but can be plotted in POST.					

V	Abbrev.	Unit	Descript.	Domain	Suffix
<sup>3</sup> Calculated for phases with magnetic contributions in an equilibrium state.					

## The u-Fraction Variable

The u-fraction is an important quantity in some single-point or stepping paraequilibrium calculations in the POLY module and in the DICTRA module. You can apply the variable in a paraequilibrium calculation to the substitutional matrix component, the substitutional alloying components or the interstitial component. The u-fraction is denoted as  $u_i$  for the  $i$ -th system component  $n$  of a whole system or of a specific phase in various equilibrium states (such as full-equilibria, partial-equilibria, para-equilibria, local-equilibria).

Generally, the u-fraction is defined as:

$$\frac{x_i}{\sum_{j \in S} x_j}$$

The sum of  $x_j$  in the denominator is calculated for the substitutional matrix element and all substitutional alloying element in the whole system or in a specific phase. The variable  $x_i$  in the numerator stands for the mole-fraction of the  $i$ -th component in the whole system or in the specific phase.

## Suffixes

Suffixes may be appended to all extensive variables and to some intensive variables. Some suffixes can be used to enter the value of variables in normalized form. These are referred to as normalizing suffixes. If the variable that you create with a normalizing suffix is based on a state variable that can be set as a condition in POLY, then the normalized variable can also be set as a condition in POLY.

The normalizing suffixes are M, W, V and F. There is also a reference state suffix  $R$ , which you can use if you want the value of a thermodynamic variable to be calculated with respect to a reference state that have previously set.

### Normalizing Suffixes

When variables that express system and phase quantities are normalized, the following general rules are used:

- System quantities are normalized by the total system size (in terms of N, B or V).
- Phase quantities are normalized by the phase amount [in terms of NP(ph), BP(ph) or VP (ph)].

The normalized quantities of G(ph), A(ph), U(ph), H(ph), S(ph) and V(ph) are calculated according to the thermodynamic model used for the phase (e.g. GM(ph), AM(ph), UM(ph), HM(ph), SM(ph) and VM(ph)).



These quantities are calculated using the first derivatives of the Gibbs energy expressed for the phase with respect to the current composition of the system.

The tables describe the normalizing suffixes for the different state variables.

### G, A, U, H, S and V of a Whole System

Suffix	Description	Example(s)
M (per mole)	First derivative of the variable with regard to the total system size in terms of N.	GM is the Gibbs energy per mole of the system (J/mol). $GM = \partial G / \partial N$
W (per mass in gram)	First derivative of the variable with regard to the total system size in terms of B.	GW is the Gibbs energy per mass of the system (J/g). $GW = \partial G / \partial B$
V (per volume in m <sup>3</sup> )	First derivative of the variable with regard to the total system size in terms of V. VV does not have to be evaluated.	GV is the Gibbs energy per volume of the system (J/m <sup>3</sup> ). $GV = \partial G / \partial V$

### G(ph), A(ph), U(ph), H(ph), S(ph) and V(ph) of a Phase

Suffix	Description	Example(s)
M (per mole)	First derivative of the variable with regard to the phase amount in terms of NP(ph).	GM is Gibbs energy of the phase per mole of the phase (J/mol). $GM(ph) = \partial G(ph) / \partial NP(ph)$
W (per mass in gram)	First derivative of the variable with regard to the phase amount in terms of BP(ph).	GW is Gibbs energy of the phase per mass of the phase (J/mol). $GW(ph) = \partial G(ph) / \partial BP(ph)$
V (per volume in m <sup>3</sup> )	First derivative of the variable with regard to the phase amount in terms of VP(ph). VV(ph) does not have to be evaluated.	GV is Gibbs energy of the phase per volume of the phase (J/mol). $GV(ph) = \partial G(ph) / \partial VP(ph)$
F (per mole formula unit)	First derivative of the variable with regard to the phase amount in terms of NP(ph) and NA (NA is the total atomic number in the phase formula)	GF(ph) is the Gibbs energy of the phase per formula unit of the phase (J/mol). $GF(ph) = \partial G(ph) / \partial NP(ph) * NA$

### DG(ph) of a Phase

Suffix	Description	Example(s)
M (per mole)	<p>Theoretically, the first derivative of the variable with regard to the phase amount in terms of NP(ph). Since DG(ph) is not directly calculated, the second derivative of the Gibbs energy expressed for the phase in question with respect to the current compositions in the equilibrium state of the system is calculated instead.</p> <p>DGM(ph) cannot not be set as a condition since it is only calculated under a certain type of equilibrium state.</p>	<p>DGM(ph) is driving force for precipitation of the phase per mole of components.</p> $DGM(ph) = \partial DG(ph) / \partial NP(ph)$
W (per mass in gram)	<p>Theoretically, the first derivative of the variable with regard to the phase amount in terms of BP(ph). Since DG(ph) is not directly calculated, the second derivative of the Gibbs energy expressed for the phase in question with respect to the current compositions in the equilibrium state of the system is calculated instead.</p> <p>DGW(ph) cannot not be set as a condition since it is only calculated under a certain type of equilibrium state.</p>	<p>DGW(ph) is driving force for precipitation of the phase per mass of components.</p> $DGW(ph) = \partial DG(ph) / \partial BP(ph)$
V (per volume in m <sup>3</sup> )	<p>Theoretically, the first derivative of the variable with regard to the phase amount in terms of VP(ph). Since DG(ph) is not directly calculated, the second derivative of the Gibbs energy expressed for the phase in question with respect to the current compositions in the equilibrium state of the system is calculated instead.</p> <p>DGV(ph) cannot not be set as a condition since it is only calculated under a certain type of equilibrium state.</p>	<p>DGV(ph) is driving force for precipitation of the phase per volume of components.</p> $DGV(ph) = \partial DG(ph) / \partial VP(ph)$
F (per mole formula unit)	<p>Theoretically, the first derivative of the variable with regard to the phase amount in terms of NP(ph) and NA (NA is the total atomic number in the phase formula). Since DG(ph) is not directly calculated, the second derivative of the Gibbs energy expressed for the phase in question with respect to the current compositions in the equilibrium state of the system is calculated instead.</p> <p>DGF(ph) cannot not be set as a condition since it is only calculated under a certain type of equilibrium state.</p>	<p>DGF(ph) is driving force for precipitation of the phase per formula unit of components.</p> $DGF(ph) = \partial DG(ph) / \partial NP(ph) * NA$

## N and B of a System

Suffix	Description	Example(s)
M (per mole)	First derivative of the variable with regard to the total system size in terms of N. NM does not have to be evaluated. BM cannot be set as a condition.	BM is mass (gram) of components per mole of the system (g/mol). $BM = \partial B / \partial N$
W (per mass in gram)	First derivative of the variable with regard to the total system size in terms of B. BW does not have to be evaluated. NW cannot be set as a condition.	NW is mole number of components per mass of the system (mol/g). $NW = \partial N / \partial B$
V (per volume in m <sup>3</sup> )	First derivative of the variable with regard to the total system size in terms of V. BV is the density of the entire system.	NV is mole number of components per volume of the system (mol/m <sup>3</sup> ). $NV = \partial N / \partial V$

### N (comp) and B(comp) of a Component in the System

Suffix	Description	Example(s)
M (per mole)	First derivative of the variable with regard to the total system size in terms of N. BM(c) cannot be set as a condition.	NM(comp) is mole number of a component per mole of the system (mole fraction, that is, X (comp)). $NM(comp) = \partial N(comp) / \partial N$
W (per mass in gram)	First derivative of the variable with regard to the total system size in terms of B. NW(c) cannot be set as a condition.	BW(comp) is mass (gram) of a component per mass of the system (mass fraction, that is, W (comp)). $BW(comp) = \partial B(comp) / \partial B$
V (per volume in m <sup>3</sup> )	First derivative of the variable with regard to the total system size in terms of V.	NV(comp) is mole number of a component per volume of the system (mol/m <sup>3</sup> ). $NV(comp) = \partial N(comp) / \partial V$

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

Suffix	Description	Example(s)
M (per mole)	<p>BPM(ph) and VPM(ph): First derivative of the variable with regard to the phase amount in terms of NP(ph).</p> <p>NPM(ph): First derivative of the variable with regard to the total system size in terms of N.</p>	<p>BPM(ph) is mass (gram) of a phase per mole of the phase in the system (g/mol).</p> $\text{BPM(ph)} = \partial \text{BP(ph)} / \partial \text{NP(ph)}$ <p>NPM(ph) is mole number of a phase per mole of the system (mole fraction).</p> $\text{NPM(ph)} = \partial \text{NP(ph)} / \partial \text{N}$
W (per mass in gram)	<p>NPW(ph) and VPW(ph): First derivative of the variable with regard to the phase amount in terms of BP(ph).</p> <p>BPW(ph): First derivative of the variable with regard to the total system size in terms of B.</p>	<p>VPW(ph) is volume (m<sup>3</sup>) of a phase per mass of the phase in the system (m<sup>3</sup>/g)</p> $\text{VPW(ph)} = \partial \text{VP(ph)} / \partial \text{BP(ph)}$ <p>BPW(ph) is mass (gram) of a phase per mass of the system (mass fraction)</p> $\text{BPW(ph)} = \partial \text{BP(ph)} / \partial \text{B}$
V (per volume in m <sup>3</sup> )	<p>NPV(ph) and BPV(ph): First derivative of the variable with regard to the phase amount in terms of VP(ph).</p> <p>VPV(ph): First derivative of the variable with regard to the total system size in terms of V.</p>	<p>NPV(ph) is mole number of a phase per volume of the phase in the system (mol/m<sup>3</sup>).</p> $\text{NPV(ph)} = \partial \text{NP(ph)} / \partial \text{VP(ph)}$ <p>VPV(ph) is volume (m<sup>3</sup>) of a phase per volume of the system (volume fraction).</p> $\text{VPV(ph)} = \partial \text{VP(ph)} / \partial \text{V}$

### N(ph,comp) and B(ph,comp) of a Component in a Phase

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

Suffix	Description	Example(s)
V (per volume in m <sup>3</sup> )	First derivative of variable with regard to the phase amount in terms of VP(ph) of the phase.	NV(ph,comp) is mole number of a component per volume of a phase (mol/m <sup>3</sup> ). NV(ph,comp) = $\partial N(\text{ph,comp}) / \partial VP(\text{ph})$

### The Reference State Suffix R

You can use the reference state suffix **R** for some thermodynamic variables to calculate their value with respect to a reference state that you have previously set for a system component with the [SET\\_REFERENCE\\_STATE on page 169](#) command in POLY (or in a response-driven modules such as the POURBAIX module). The value of energy-related variables that are used with the **R** suffix depends on the reference states of all the components in the defined system.



It is possible to use an **R** suffix on all compositional extensive state variables as well, but the value of the state variable is always the same, with or without the suffix.

If the reference state for a system component is the default reference state (the stable reference state (SER) which is defined in a Thermo-Calc database), then MUR(comp)= MU(comp), ACR(comp)= AC(comp) and LNACR(comp)= LNAC(comp).

In the case of some thermodynamic variables, you can also use the **R** suffix to express chemical potentials and activities of species relative to some single-substitutional-lattice solution phases (such as aqueous solution, gaseous mixture, metallic liquid solution, slag mixture or MO solid solution). These state variables are MU(sp,ph), MUR(sp,ph), AC(sp,ph), ACR(sp,ph), LNAC(sp,ph) and LNACR(sp,ph).

The reference states and standard states of various solution species are pre-defined for some solution phases in some databases. For all solution species in any solution model in any database, it is always the case that MUR(sp,ph)= MU(sp,ph), ACR(sp,ph)= AC(sp,ph) and LNACR(sp,ph)= LNAC(sp,ph).

## Derived Variables and Partial Derivatives

Many derived variables can be obtained easily by using partial derivatives of state variables, such as heat capacity, thermal expansivity, isothermal compressibility, among others.

Derivatives of state variables can be defined or evaluated by putting a dot (.) between two state variables. The variable after the dot must be a condition that you have set when you defined your system. For example, the heat capacity (at constant pressure or volume) of a system is the partial derivative of the state variable enthalpy with respect to temperature. To evaluate this derivative, use the designation HM.T, where temperature is a state variable that you have set already.

Any partial derivative of a state variable with respect to another can be defined or evaluated as a derived variable by using the dot (.) notation.

### Derived Variables Dot Notation Examples

The following table shows some examples:

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

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

## Defining New Derived Variables and Functions

You can define additional derived variables or functions based on a state variable by using [ENTER\\_SYMBOL](#) on page 195. Any derived variable or function must have a unique name that starts with a letter and has a maximum number of eight characters. These characters can include both uppercase and lowercase letters, numerical digits and the underscore (\_). No other characters are allowed.

The difference between new derived variables introduced with the ENTER\_SYMBOL command and new functions introduced with the same command is as follows. Whenever Thermo-Calc calculates the value of a function (as part of an equilibrium calculation for example), all functions related to the defined system is evaluated. An entered derived variable, on the other hand, is only evaluated when it is defined and when it is re-evaluated with [EVALUATE\\_FUNCTIONS](#) on page 155.

## Derived Variables for Aqueous Solutions

Standard state variables used for other phases can be directly applied to the aqueous solution phase. In addition, there are pre-defined derived variables for the aqueous solution phase in particular.

Examples of predefined derived variables for the aqueous solution phase are listed and briefly described in the following tables. Some derived variables for a gaseous mixture phase are also shown. This is because EOS (Equation of State) expressions, standard thermodynamic properties and transport properties of the pure solvent H<sub>2</sub>O are also expressions and properties of the pure gaseous species H<sub>2</sub>O.

### For Aqueous Solution Phase

Name	Abbrev.	Units	Description	Comments
pH	PH	N/A	Acidity	of the aqueous solution phase $\text{pH} = -\log_{10}(\text{AC}(\text{H}^+)) = -\log_{10}(\text{ACR}(\text{H}^+, \text{AQ}))$
Eh	EH	V, mV	Hypothetical electric potential	of the aqueous solution phase $\text{Eh} = u(\text{ZE})/96485.309$
Pe	PE	N/A	Logarithm of the hypothetical electron activity	of the aqueous solution phase $\text{pe} = u(\text{ZE})/(2.3025851 \cdot \text{RT})$
Ah	AH	kJ, kcal	Thermodynamic affinity per electron	of a redox couple wrt the standard hydrogen electrode in the aqueous solution phase $\text{Ah} = u(\text{ZE})$
yw	YH2O	N/A	Mole fraction	of the solvent H2O in the aqueous solution phase $\text{YH2O} = \text{Y}(\text{AQ}, \text{H2O})$
Nw	AH2O	mole	Mole number	of 1.0 kg of solvent H2O $\text{AH2O} = 55.508435$
Nsp	NSH2O	mole	Mole number, $\text{NS}(\text{AQ}, \text{H2O})$	of the solvent (H2O) in the aqueous solution phase $\text{NS}(\text{AQ}, \text{H2O}) = \text{YH2O} \cdot \text{NP}(\text{AQ})$
	NS#		Mole number, $\text{NS}(\text{AQ}, \text{sp})$	of a solute species in the aqueous solution phase $\text{NS}(\text{AQ}, \text{sp}) = \text{Y}(\text{AQ}, \text{sp}) \cdot \text{NP}(\text{AQ})$
M	ML#	mol/kg_H2O	Molality, $\text{ML}(\text{AQ}, \text{sp})$	of a solute species in the aqueous phase $\text{ML}(\text{AQ}, \text{sp}) = \text{Y}(\text{AQ}, \text{sp}) \cdot \text{AH2O} / \text{YH2O}$



Name	Abbrev.	Units	Description	Comments
m*	TIM	equivalent molality	Total molality	of all solute species in the aqueous solution phase TIM = sum[ML(AQ,sp)]ions + sum[ML(AQ,sp)]complexes
mt	TIC#	equivalent molality	Total ionic concentration, TIC (AQ,sp)	of a cation I in the aqueous phase TIC(AQ,spI) = sum[ML(AQ,spJ)*V(spI-in-spJ)]
I	ISTR	N/A	Ionic strength	of the aqueous solution phase ISTR=1/2*sum[ML(AQ,sp)*Z(AQ,sp)**2]
$\gamma$	RCH2O	N/A	Activity coefficient, RC(H2O,AQ)	of the solvent (H2O) RC(H2O,AQ) = ACR(H2O,AQ)/YH2O
	RC#		Activity coefficient, RC(sp,AQ)	of a solute species RC(sp,AQ) = ACR(sp,AQ)/Y(AQ,sp)*YH2O
$\alpha_i$	AIH2O	N/A	Activity, AI(H2O,AQ)	of the solvent (H2O), AI(H2O,AQ) = ACR(H2O,AQ)
	AI#		Activity, AI(sp,AQ)	of a solute species related to the aqueous solution phase, AI(sp,AQ) = ACR(sp,AQ)*AH2O
	LogAI#		Log10 Activity, LogAI(H2O,AQ), LogAI(sp,AQ)	of the solvent or a solute species related to the aqueous solution phase in common logarithm, LogAI(H2O,AQ) = log10 [AI(H2O,AQ)]

Name	Abbrev.	Units	Description	Comments
				$\text{LogAl}(\text{sp}, \text{AQ}) = \log_{10}[\text{Al}(\text{sp}, \text{AQ})]$
$\alpha_w$	AW	N/A	Activity	of H <sub>2</sub> O in the aqueous solution phase $\text{AW} = \text{ACR}(\text{H}_2\text{O}, \text{AQ})$
$\phi$	OS	N/A	Osmotic coefficient	of aqueous solution phase $\text{OS} = -55.508435 * \ln \text{AW} / \text{TIM}$
At1	AT1	equil_mol/kg_H2O	Titration alkalinity (definition 1)	of the aqueous solution phase Generally defined as the equivalent molality of carbonate and bicarbonate at the methyl orange endpoint (pH=4.5).
At2	AT2	equil_mol/kg_H2O	Titration alkalinity (definition 2)	of the aqueous solution phase Generally defined as the equivalent molality of carbonate and bicarbonate, plus sulfide, at the methyl orange endpoint (pH=4.5).

### For Gaseous Mixture Phase

Name	Abbrev.	Units	Description	Comments
$\gamma$	RA#	N/A	Activity coefficient, $\text{RA}(\text{sp}, \text{GAS})$	of a gaseous species in the gaseous mixture $\text{RA}(\text{sp}, \text{GAS}) = \text{function}(\text{Y}, \text{T}, \text{P})$
$\gamma^*$	RF#	N/A	Fugacity coefficient, $\text{RF}(\text{sp}, \text{GAS})$	of a pure gaseous species under TP $\text{RF}(\text{sp}, \text{GAS}) = \text{function}(\text{T}, \text{P}/\text{V})$
F	FUG#	pa, bar, psi	Fugacity, $\text{FUG}(\text{sp}, \text{GAS})$	of a gaseous species in the gaseous mixture $\text{FUG}(\text{sp}, \text{GAS}) = \text{RA}(\text{sp}, \text{GAS}) * \text{RF}(\text{sp}, \text{GAS}) * \text{Y}(\text{GAS}, \text{sp}) * \text{P}$

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

## Defining New Derived Variables for Aqueous Solutions

You can define many different additional derived variables and functions. For instance, the partition coefficient of a component between two phases is defined as follows:

$$Pc<name> = X(phase1, component) / X(phase2, component)$$

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

$$Rc<name> = ACR(component) / X(component)$$

The activity coefficient of a species in a solution phase depends on which model definitions on the reference states that are used and it depends on the standard states for the species. If the standard state of a species is defined to be the same as the pure species in a substitutional phase, then the activity coefficient of the species can be calculated as:

$$RC<name> = ACR(species, phase) / Y(phase, species)$$

In some cases, there are more than one sublattice in the phase and the reference states for the phase species cannot be presented by the pure species, as in the case of C in FCC [(Fe)1(C,N,VA)1], where the model may end at fifty percent C and fifty percent Fe. In those cases, the chemical potential and activity of all phase constituents is not well defined and you cannot properly define the activity coefficients of the species in the phase.

For an aqueous solution phase, no matter what model is used, the reference state and standard state for both the solvent and solutes are defined in a special way in the Thermo-Calc software. The reference state for the solvent is set as pure water, the same as its standard state (according to Raoult's Law). The standard state for a solute species is set the hypothetical solute species, whilst its reference state is defined as the hypothetical state at unit molality (one mole dissolved into 1.0 kg of solvent) but in which the environment of each molecular is the same as at infinite dilution (according to Henry's Law). Under these definitions, the activity coefficients for solvent species can be calculated as follows:

$$RC<H2O> = ACR(H2O, aqueous) / Y(aqueous, H2O)$$

The coefficients for the solute species can be calculated as follows:

$$RC<spec> = AI(species, aqueous) / ML(aqueous, species) \\ = ACR(species, aqueous) / Y(aqueous, species) * Y(aqueous, H2O)$$

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

## Thermodynamic Variables and Wildcard Characters

The ACR (species, phase) and the MUR (species, phase) quantities can only be appropriately and meaningfully applied to substitutional solution phases (such as GAS, AQUEOUS, LIQUID) and to solution

phases without an interstitial sublattice set. This means that the wild card characters \* and \$ normally don't work properly for the activity and/or chemical potential properties.

For example, do not use `ACR(*,*)` or `MUR(*,*)` for all the species relative to all phases, nor `ACR(*,phase)` or `MUR(*,phase)` for all the species relative to a specific phase, nor `ACR(species,*)` or `MUR(species,*)` for a specific species relative to all phases.

Instead, use specific names for species and (applicable) phase, as in the following examples:

```
show_value acr(fe+2,aqueous)Lists activity of the Fe+2 species in AQUEOUS solution
phase
show_value mur(c2,gas)Lists chemical potential of the C2 species in GAS mixture phase
set_axis_var y ac(o2,gas)Sets activity of the O2 species in GAS mixture phase as Y-
axis
```

## Units of State Variables and Derived Variables

The units for the state variables in the Units column in the table in [User-Specified Units below](#) are the SI units that are used in the POLY module. However, in the POST module, you can both use pre-defined symbols and define your own symbols which are based on state variables and derived variables. By doing this, you can express the value of the thermodynamic variables in non-default units. The following topic briefly describes how you can create your own symbols and suggests expressions that you can use to convert default units into other standard units which are not default units in Thermo-Calc.

The topic [Examples of User-Defined Units on the next page](#) describes some variables of specific species in a phase and the units in which they are expressed. These variables are not used in POLY or POST, but in the GIBBS, DATA, PARROT and ED\_EXP modules.

### User-Specified Units

You do not always need to use the default units for variables. Using [ENTER\\_SYMBOL on page 195](#), you can convert the value of variable from the default unit to your preferred unit. (Some response-driven modules also allow you to set conditions in non-default units.) User-defined symbols in the form of functions can be used for plotting in the POST module, but they cannot be used as conditions in POLY. User defined symbols in the form of variables can be used as conditions.

For example, if you want pressure to be plotted in bar rather than Pa, then you define the following function PB:

```
ENTER_SYMBOL FUNCTION PB = P/1E5 ;
```

If you wanted heat capacity of a system to be shown as in terms of J/mol/K, then you can define the following function Cp:

```
ENTER_SYMBOL FUNCTION CP = HM.T ;
```

If the variable you want to convert is a function of one or more derivatives, then you must enter the symbol as a variable rather as a function. For instance, a symbol expressing heat capacity of a system in a unit of cal/mol/K can be defined as the following variable Cp2:

```
ENTER_SYMBOL VARIABLE CP2 = HM.T/4.1858 ;
```



Also see [Examples of User-Defined Units](#) below for information about entering conventional functions and the associated units.

## Examples of User-Defined Units

The following tables give examples of expressions you can use to enter symbols. This enables you to show the values of thermodynamic variables in a variety of units.



[Units of State Variables and Derived Variables](#) on the previous page and [User-Specified Units](#) on the previous page



You can also use thermodynamic variables with normalizing suffixes in the expression when you enter a symbol. However, the tables do not have examples of these expressions.

In the expressions these are defined as follows:

- $i$  is for an auxiliary index or letter that corresponds to the component  $c$
- $j$  is for an auxiliary index or letter that corresponds to the phase  $ph$ , and
- $ij$  stands for an auxiliary index or letter that corresponds to the component  $c$  in the phase  $ph$ .

## Intensive and Extensive Variables of a Defined System

Quantity	Suggested name and expression	Unit
<i>For intensive variables of a defined system</i>		
Temperature	TempC = T-273.15	Celsius (C)
	TempF = 1.8*T-459.67	Fahrenheit (F)
	TempF = 1.8*TempC+32	
Pressure	PB = P/1E5	bars (bar)
	PKb = P/1E8	kilobars (kbar)
	PAtm = P/101325	atmosphere (atm)
	PSI = P/6894.76	pounds/sq. inch (psi)
	PIHg = P/3342.11	inches of Hg
	PTor = P/133.322	Tors (millimeters of Hg)

Quantity	Suggested name and expression	Unit
<i>For extensive variables of a defined system</i>		
Amount	BKg = $1\text{E-}3 \cdot B$	kilograms (kg)
	BTon = $1\text{E-}6 \cdot B$	tons
Volume	VDM = $1\text{E-}3 \cdot V$	cubic decimeters (dm <sup>3</sup> , l)
	VCM = $1\text{E-}6 \cdot V$	cubic centimeters (cm <sup>3</sup> )
	VMM = $1\text{E-}9 \cdot V$	cubic millimeters (mm <sup>3</sup> )
	VCI = $1.6387064\text{E-}5 \cdot V$	cubic inches (in <sup>3</sup> )
	VLi = $1\text{E-}3 \cdot V$	liters (l)
Energy	GCal = $G/4.1858$	cal
	ACal = $A/4.1858$	cal
	UCal = $U/4.1858$	cal
	HCal = $H/4.1858$	cal
	SCal = $S/4.1858$	Cal/K
Heat Capacity	Cp2 = $HM.T/4.1858$	cal/mol/K
	Cp3 = $HW.T/4.1858$	cal/g/K
	Cp4 = $HV.T/4.1858$	cal/m <sup>3</sup> /K
Thermal Expansion	A2 = $VM.T \cdot 1\text{E-}6 \cdot VM$	cm <sup>3</sup> /mol/K
	A3 = $VW.T \cdot 1\text{E-}6 \cdot VM$	cm <sup>3</sup> /g/K
Isothermal Compressibility	B2 = $-VM.P \cdot 1\text{E-}9 \cdot VM$	mm <sup>3</sup> /mol/Pa
	B3 = $-VW.P \cdot 1\text{E-}9 \cdot VM$	mm <sup>3</sup> /g/Pa

### Intensive and Extensive Variables of a System Component

Quantity	Suggested name and expression	Unit
<i>For intensive variables of a system component</i>		
Chemical Potential	MUi = $MU(c)/4.1858$	cal/mol
	MURi = $MUR(c)/4.1858$	cal/mol

Quantity	Suggested name and expression	Unit
Special quantity for aqueous solution	$pH = -\log_{10}(a_{H^+})$	dimensionless
	$E_h = MUR(ZE)/RNF$ where $RNF=96485.309$	volts (V)
<i>For extensive variables of a system component</i>		
Amount	$MFi = N(c)/N = X(c)$	dimensionless
	$MPi = N(c)/N \cdot 100$	dimensionless
	$WFi = B(c)/B = W(c)$	dimensionless
	$WPi = B(c)/B \cdot 100$	dimensionless
	$BKgi = 1E-3 \cdot B(c)$	kilograms (kg)
	$BToni = 1E-6 \cdot B(c)$	tons

### Extensive Variables of a Phase

Quantity	Suggested name and expression	Unit
Amount	$MFj = NP(ph)/N$	dimensionless
	$MPj = NP(ph)/N \cdot 100$	dimensionless
	$WFj = BP(ph)/B$	dimensionless
	$WPj = BP(ph)/B \cdot 100$	dimensionless
	$BKgj = 1E-3 \cdot BP(ph)$	kilograms (kg)
	$BTonj = 1E-6 \cdot BP(ph)$	tons
Volume	$VCMj = 1E-3 \cdot V(ph)$	cubic decimeters (dm <sup>3</sup> , l)
	$VCMj = 1E-6 \cdot V(ph)$	cubic centimeters (cm <sup>3</sup> )
	$VMMj = 1E-9 \cdot V(ph)$	cubic millimeters (mm <sup>3</sup> )
Energy	$GCalj = G(ph)/4.1858$	cal
	$ACalj = A(ph)/4.1858$	cal
	$UCalj = U(ph)/4.1858$	cal
	$HCalj = H(ph)/4.1858$	cal
	$SCalj = S(ph)/4.1858$	Cal/K

Quantity	Suggested name and expression	Unit
Driving Force	$DG2j = DGM(ph)/4.1858$	cal/mol
	$DG3j = DGW(ph)/4.1858$	cal/g
	$DG4j = DGV(ph)/4.1858$	Cal/m <sup>3</sup>
	$DG5j = DGF(ph)/4.1858$	cal/mole_formula_unit
Heat Capacity	$Cp2j = HM(ph).T/4.1858$	cal/mol/K
	$Cp3j = HW(ph).T/4.1858$	cal/g/K
	$Cp4j = HV(ph).T/4.1858$	cal/m <sup>3</sup> /K
	$Cp5j = HF(ph).T/4.1858$	cal/mole_formula_unit/K
Thermal Expansion	$A2j = VM(ph).T*1E-6*VM$	cm <sup>3</sup> /mol/K
	$A3j = VW(ph).T*1E-6*VM$	cm <sup>3</sup> /g/K
	$A4j = VF(ph).T*1E-6*VM$	cm <sup>3</sup> /mole_formula_unit/K
Isothermal Compressibility	$B2j = -VM(ph).P*1E-9*VM$	mm <sup>3</sup> /mol/Pa
	$B3j = -VW(ph).P*1E-9*VM$	mm <sup>3</sup> /g/Pa
	$B4j = -VF(ph).P*1E-9*VM$	mm <sup>3</sup> /mole_formula_unit/Pa

### Extensive Variables of a Component in a Phase

Quantity	Suggested name and expression	Unit
Amount	$MFij = N(ph,c)/NP(ph) = X(ph,c)$	dimensionless
	$MPij = N(ph,c)/NP(ph)*100$	dimensionless
	$WFi = B(ph,c)/BP(ph) = W(ph,c)$	dimensionless
	$WPij = B(ph,c)/BP(ph)*100$	dimensionless
	$BKgj = 1E-3*B(ph,c)$	kilograms (kg)
	$BTonij = 1E-6*B(ph,c)$	tons

### Intensive and Extensive Variables of a Species in a Phase



Quantity	Suggested name and expression	Unit
<i>For intensive variables of a species in a phase</i>		
Chemical Potential	MUCalij = MU(sp,ph)/4.1858	cal/mol
	MUErgij = MU(sp,ph)*1E7	cal/mol
Fugacity	FAij = AC(sp,ph)*PATM	atmosphere (atm)
	FBij = AC(sp,ph)*PB	bars (bar)
	FCij = AC(sp,ph)*PKB	kilobars (kbar)
	FTij = AC(sp,ph)*PTOR	Tors (millimeters of Hg)
ln(Fugacity)	LnFAij = LNAC(sp,ph)+LN(PATM)	atmosphere (atm)
	LnFBij = LNAC(sp,ph)+LN(PB)	bars (bar)
	LnFCij = LNAC(sp,ph)+LN(PKB)	kilobars (kbar)
	LnFTij = LNAC(sp,ph)+LN(PTOR)	Tors (millimeters of Hg)
Special quantity for aqueous solution	Alij=ACR(Fe+3,AQ)*AH2O	dimensionless
	RCij=ACR(Fe+3,AQ)*YH2O/Y(AQ,Fe+3) where AH2O=55.508435 and YH2O=Y(AQ,H2O)	dimensionless
	WRCalij = WR(AQ,sp)/4.1858 (WR(AQ,sp) is only valid for aqueous species in a system in which the AQUEOUS solution phase is considered)	cal/mol
<i>For extensive variables of a species in a phase</i>		
Special quantity for aqueous solution	MLij=Y(AQ,Fe+3)*AH2O/YH2O	molality (m)
	ISTR=1*IS1+1*IS2+1*IS3 where AH2O=55.508435, YH2O=Y(AQ,H2O) and ISn=.5*MLi*Zi**2+.5*MLj*Zj**2+.5*MLk*Zk**2	molality (m)

### Units for Variables of Specific Species in a Phase

In the GIBBS, DATA, PARROT and ED\_EXP modules, there are quantities that describe various

thermodynamic, physical, chemical and transport properties for a compound phase, and for a certain species or a given species combination in a specific solution phase. The following table describes the units for those variables.



These variables cannot be directly used in the POLY or POST modules.

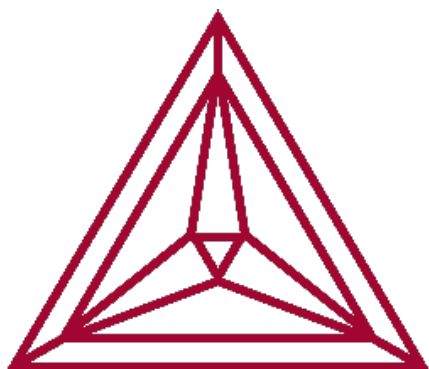
Variables	Description and unit
G(ph,sp) G(ph,sp;0) G(ph,sp1;sp2;...;0)	Gibbs energy (J/mol) of a pure substance or end-member.
G(ph,sp1,sp2,...) L(ph,sp1,sp2,...) G(ph,sp1,sp2,...;0) L(ph,sp1,sp2,...;0) G (ph,sp1,sp2,...;...;0) L (ph,sp1,sp2,...;...;0)	Zero-order interaction parameter (J/mol) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
G(ph,sp1,sp2,...;i) L(ph,sp1,sp2,...;i) G (ph,sp1,sp2,...;...;i) L (ph,sp1,sp2,...;...;i)	The ith -order interaction parameter (J/mol) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
TC(ph,sp) TC(ph,sp;0) TC(ph,sp1;sp2;...;0)	Curie temperature (K) of a pure substance or end-member.
TC(ph,sp1,sp2,...) TC(ph,sp1,sp2,...;0) TC (ph,sp1,sp2,...;...;0)	Zero-order Curie-temperature contribution (K) to a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
TC(ph,sp1,sp2,...;i) TC (ph,sp1,sp2,...;...;i)	The ith -order Curie-temperature contribution (K) to a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.

Variables	Description and unit
BMAGN(ph,sp) BMAGN(ph,sp;0) BMAGN (ph,sp1;sp2,...;0)	Bohr magneton number (dimensionless) of a pure substance or end-member.
BMAGN (ph,sp1,sp2,...) BMAGN (ph,sp1,sp2,...;0) BMAGN (ph,...;sp1,sp2,...;0)	Zero-order Bohr magneton number (dimensionless) to a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
BMAGN (ph,sp1,sp2,...;i) BMAGN (ph,sp1,sp2,...,...;i)	The ith -order Bohr magneton number (dimensionless) to a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
V0(ph,sp) V0(ph,sp;0) V0(ph,sp1;sp2,...;0)	Molar volume ( $\text{m}^3$ ) at 1 bar and reference T0 of a pure substance or end-member.
V0(ph,sp1,sp2,...) V0(ph,sp1,sp2,...;0) V0 (ph,sp1,sp2,...,...;0)	Zero-order composition-dependent molar volume ( $\text{m}^3$ ) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
V0(ph,sp1,sp2,...;i) V0 (ph,sp1,sp2,...,...;i)	The ith-order composition-dependent molar volume ( $\text{m}^3$ ) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
VA(ph,sp) VA(ph,sp;0) VA(ph,sp1;sp2,...;0)	Integrated thermal expansivity ( $\text{m}^3/\text{mol/K}$ ) of a pure substance or end-member.
VA(ph,sp1,sp2,...) VA(ph,sp1,sp2,...;0) VA (ph,sp1,sp2,...,...;0)	Zero-order composition-dependent thermal expansivity ( $\text{m}^3/\text{mol/K}$ ) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.

Variables	Description and unit
VA(ph,sp1,sp2,...;i) VA (ph,sp1,sp2,...;...;i)	The ith -order composition-dependent thermal expansivity ( $\text{m}^3/\text{mol/K}$ ) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
VC(ph,sp) VB(ph,sp;0) VB(ph,sp1;sp2;...;0)	Isothermal compressibility ( $\text{m}^3/\text{mol/Pa}$ ) of a pure substance or end-member.
VC(ph,sp1,sp2,...) VB(ph,sp1,sp2,...;0) VB (ph,sp1,sp2,...;...;0)	Zero-order composition-dependent isothermal compressibility ( $\text{m}^3/\text{mol/Pa}$ ) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
VC(ph,sp1,sp2,...;i) VB (ph,sp1,sp2,...;...;i)	The ith -order composition-dependent isothermal compressibility ( $\text{m}^3/\text{mol/Pa}$ ) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
VK(ph,sp) VB(ph,sp;0) VB(ph,sp1;sp2;...;0)	High-pressure fitting parameter ( $\text{m}^3/\text{mol}$ ) of a pure substance or end-member.
VK(ph,sp1,sp2,...) VB(ph,sp1,sp2,...;0) VB (ph,sp1,sp2,...;...;0)	Zero-order composition-dependent high-pressure fitting parameter ( $\text{m}^3/\text{mol}$ ) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
VK(ph,sp1,sp2,...;i) VB (ph,sp1,sp2,...;...;i)	The ith -order composition-dependent high-pressure fitting parameter ( $\text{m}^3/\text{mol}$ ) of a specified binary, ternary or higher-order interactions on a certain sublattice site in a solution phase.
WR(ph,sp) WR(ph,sp;0)	Standard Born function ( $\text{J/mol}$ ) of a specific aqueous species in the AQUEOUS solution phase (always with a single sublattice) under the reference-state temperature and pressure.

# **Data Optimization User Guide**

**Thermo-Calc Version 2016a**



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# Introduction

In this section:

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<i>Introduction to Data Optimization</i> .....	3
<i>Data Optimization</i> .....	3
<i>The Least-Squares Method</i> .....	4
<i>The CALPHAD Approach</i> .....	4

## Introduction to Data Optimization

This user guide describes the basic idea behind data optimization, contains brief descriptions of the modules and file types that you work with while doing your optimization, as well as rough outline of overarching workflow that you typically follow when working with optimization.

This guide assumes that you are familiar with using the Thermo-Calc Console Mode. It also assumes that you understand the principles of thermodynamics and are familiar with the theoretical foundations of computational thermodynamics.



Also see the *Thermo-Calc Console Mode Command Reference* included with this documentation set, which has information about all the commands available in the Thermo-Calc Console Mode, including PARROT and ED\_EXP. Note that the commands listed under PARROT and ED\_EXP are only commands that are specific to PARROT and/or ED\_EXP. These modules also contain some commands that are also available in POLY.



*Example 36* in the *Console Mode Examples Guide*. It is a detailed example of assessment and optimization in Thermo-Calc.

## Data Optimization

In a thermodynamic database, each phase in a system is characterised using a mathematical model of its Gibbs energy. The Gibbs energy of a phase depends on various state variables. It can be defined individually even in a heterogeneous system with many stable phases since the properties of one phase are completely independent of the properties of the other phases in the system. In most alloy systems, the thermodynamic properties of a phase can be modelled by expressing how the Gibbs energy depends on temperature and composition. State variables such as pressure, volume or entropy can also serve as parameters in the Gibbs energy expression. The Gibbs energy of the whole system is the sum of the products of the Gibbs energy of each phase multiplied by the amount of that phase.

How the Gibbs energy of the phase varies with various state variables is determined by a mathematical model and how various adjustable parameters of the model is set. By optimizing these parameters, you can calculate the thermodynamic properties of a system under various conditions (by calculating phase diagrams for example). The thermodynamic properties themselves are functions of temperature, pressure or composition. They include, among other properties, standard enthalpy of formation, entropy, heat capacity, molar volume, thermal expansivity, compressibility and Curie temperature for magnetic transformations.

Data optimization is about adjusting the model parameters so that calculated equilibria fit well with experimental data. An important part of a data optimization is therefore collecting and assessing available experimental and theoretical information about phase equilibria and thermochemical properties of a system.

When you optimize the parameters of the model of a phase, you put what is called optimizing variables into the Gibbs energy expressions of those parameters. During the optimization, the values of these

variables are varied in order to find a fit between the calculated equilibria and the experimental data that you base the optimization on. Once you have settled on a Gibbs energy expression for a certain parameter of a phase of the element, then you must stick to this expression in all future optimizations involving the element. If you do not do this, then you must re-optimize all previous systems that involve this element when the expression is changed.

The Thermo-Calc software allows you to optimize parameters that characterize not only binary systems, but also ternary system and systems of even higher orders. You can even optimize parameters that characterise systems of different orders at the same time.

## The Least-Squares Method

Data optimization in Thermo-Calc is based on the least-squares method for fitting values calculated on the basis of a model with observed quantities. The software is accordingly trying to find the optimizing variable values that lead the minimized sum of the squares of the differences between the calculated values and the observed quantities (that is, of the errors or residuals).

The least-squares method works best under the following conditions:

- The observed quantities have a Gaussian probability distribution.
- The observed quantities are only subject to random errors.
- The different observations (experiments) are uncorrelated
- The standard deviation of each observation can be estimated.
- The number of observations is large.
- The models used give precise predictions.

Of course, these conditions are usually not all met in a normal thermodynamic assessment. But even in non-ideal conditions, there is no known method that works better than the least-squares method.

## The CALPHAD Approach

The data optimization functionality in Thermo-Calc works according to the CALPHAD approach to computational thermodynamics. This approach builds on the development of models that accurately represent thermodynamic properties for various phases. These models enable you to predict the thermodynamic properties of multicomponent systems-based data concerning binary and ternary subsystems. The predictions can take many factors into accounts, such as, for example, crystallography, type of bonding, order-disorder transitions and magnetic properties.

CALPHAD is originally an abbreviation of *CAL*culat*ion of PH*ase *D*iagrams, but as the approach has expanded in scope, it now stands for *computer coupling of phase diagrams and thermochemistry*.

### References

For in-depth information about CALPHAD as well as data optimization, see *Computational*



*Thermodynamics – The Calphad Method* by Hans Leo Lukas, Suzana G. Fries and Bo Sundman (Cambridge University Press, 2007). CALPHAD was given its first general description in *Computer Calculations of Phase Diagrams* by Larry Kaufman and Harold Bernstein (Academic Press, 1970). The book contains some case studies of optimizations using Thermo-Calc.

Information about the concept of ‘lattice stability’ (which is important for the development of multicomponent thermodynamic databases) can also be found in the paper *Hume-Rothery and Calphad Thermodynamics* by Larry Kaufman, published in *Calphad and Alloy Thermodynamics*, edited by Patrice E.A. Turchi, Antonios Gonis, Robert Shull (The Minerals, Metals & Materials Society, 2002), pp. 3-19.

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## Working with Data Optimization in Thermo-Calc

In this section:

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<i>Data Optimization in Thermo-Calc</i> .....	7
<i>Data Optimization Workflow</i> .....	7
<i>The PARROT Module</i> .....	8
<i>The EDIT_EXPERIMENTS Module</i> .....	8
<i>Data Optimization in Other Modules</i> .....	9
<i>Optimization File Types</i> .....	9
<i>Optimization Workspaces</i> .....	10
<i>Method for Optimization and Simulation</i> .....	10

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## Data Optimization in Thermo-Calc

The actual performance of the optimization of a system is primarily done in the PARROT module, and in its sub-module ED\_EXP. The POLY and POST modules are used to calculate and plot property or phase diagrams based on the optimized variables. This allows you to visually assess how good a fit you have achieved between your calculated results and your experimental data.

The end result of a successful optimization is typically an updated Thermo-Calc database file (with filename extension \*.TDB) or a new database file.

### Data Optimization Workflow

When you carry out an optimization using Thermo-Calc, you typically follow a workflow as outlined below.

1. Collect experimental data about your system from various sources such as journal articles and reports.
2. Create a POP-file in which you enter the experimental data you have collected.
3. Create a setup macro file in which you define your system and the variables you want to optimize. A useful general procedure is to first find a minimum set of variables that allows you to calculate most of the experiments.
4. Run the setup macro file.
5. Compile your POP-file. This file often contains errors, which need to be corrected, and the file recompiled several times before the compilation is completed without errors.
6. In the ED\_EXP module, check that the experiments in your POP-file reach equilibrium with reasonable results. If any experiments do not reach equilibrium with reasonable results, then try changing the starting values on equilibrium conditions (such as composition) to see whether the equilibrium can be computed after all. If this does not work, then you can temporarily exclude the experiment from the optimization. At a later stage in the optimization, when the optimizing variables have different values, you can check whether the experiments can be computed with reasonable results.
7. Back in the PARROT module, run the first optimization cycle and evaluate the feedback in the console. You can also plot diagrams in the POLY module that allow you to visually inspect the fit between calculated optimization results and the experimental data. If you are not satisfied with the fit, then enter the ED\_EXP module again and adjust the weights of the experiments in a way that is likely to improve the fit and run another optimization cycle. Reiterate until you are satisfied with the fit.
8. Once you get the optimization stable and smooth with the minimum set of variables chosen in step 3 above, try using different sets of variables to see whether improvements are possible.

9. When you are satisfied with the fit between calculated results and experimental data with your final set of optimizing variables, update your setup file and POP-file. In the setup file, enter the calculated optimizing variable values as the variables' start values. In the POP-file, enter the final weights of the experiments. With these files updated, you can easily regenerate the parameter values of your optimized system. Having the files updated also makes it easier to optimize the system again in light of new data or new theoretical models.
10. Finally, update the database with your calculated results or create a new database with information about the system that you have optimized.

## The PARROT Module

The PARROT module consists of a comprehensive subroutine package for data evaluation of thermodynamic model parameters from experimental data. The module has 99 variables that you can use for optimization and the module can handle a thousand experimental measurements in an optimization. However, there are limits on the simultaneous numbers of variables and experiments. These limits are listed at each optimization.



The PARROT module is part of the Thermo-Calc software. The module is not included in the software development kits TQ-Interface, TC-API or TC-Toolbox for MATLAB®.

The experimental data is entered and edited in a sub-module of PARROT: *The EDIT\_EXPERIMENTS Module* below.

## The EDIT\_EXPERIMENTS Module

The EDIT\_EXPERIMENTS module, or ED\_EXP for short, is used for entering, evaluating and editing experimental data. To enter the module, go to *The PARROT Module* above and then issue the command *EDIT\_EXPERIMENTS* on page 95.

Since ED\_EXP uses the POLY module for doing equilibrium calculations of experimental data points, many POLY commands are also available in the ED\_EXP module. However, the commands may work somewhat differently in the two modules. There are also unique ED\_EXP commands which are not found in POLY.

When you execute ED\_EXP commands, the PARROT workspace is modified. However, note that you must always first use *READ\_WORKSPACES* on page 160 in ED\_EXP before doing anything in the module. The command loads the experimental data that you are going to work with during the optimization. Furthermore, before leaving ED\_EXP you must use *SAVE\_WORKSPACES* on page 30 or the results of your work in the ED\_EXP module is lost.

## Data Optimization in Other Modules

All kinds of thermodynamic data, calculated equilibrium states or dynamic parameters are transferred back and forth between the PARROT and the GIBBS module as well between these and the POLY module. Whenever an optimization run is performed, PARROT calls the GIBBS module for stored system definition data and model parameters.

In Thermo-Calc, the GIBBS module (the Gibbs Energy System) handles the models of the various phases that can form in a multicomponent system. It stores thermodynamic data and performs various Gibbs energy equilibrium calculations. It contains subroutines to analytically calculate the first and second partial derivatives of integral Gibbs energy with respect to any set of variables. Many thermodynamic models for various types of substances are implemented in the module. Some commands that are available in the PARROT module are also available in the GIBBS module.


In the GIBBS module, parameters of the Gibbs energy models are referred to as *TP-functions*.

PARROT calls the POLY module for equilibrium calculations. The POLY module is used for calculating and storing complex heterogeneous equilibria.

## Optimization File Types

These are the important files you work with when optimizing.

File type	Description
POP-file	The POP-file (Parrot OPTimization file) is the file that contains all the experimental data that you use for optimizing Gibbs energy values for your system. The POP-file is a plain text file that contains ED_EXP commands. By default, the file has the filename extension *.POP in Thermo-Calc.
Setup file	The setup file is a Thermo-Calc macro file (*.TCM). This file typically contains commands that define your system, opens the PARROT workspace (and associated GIBBS and POLY workspaces) and sets optimizing variables.
Other macro files	It is often useful to have other macro files than the setup file at hand while you are doing your optimization. For example, it is convenient to have a macro file that automatically plots phase diagrams or other diagrams based on the latest values of your optimizing variables. An optimization process typically involves many optimization cycles, so this operation needs to be done many times during a typical optimization.
Workspace files	The PARROT module has its own workspace with dynamic memories, similar to the workspaces of POLY and GIBBS. It is stored and updated in a PARROT workspace file with the filename extension *.PAR. The workspace file is a binary file whose format is hardware dependent. This means that the format is unique for each type of CPU. Hence, a workspace file saved on a computer with one type of CPU cannot be used on a computer with another type of CPU.

File type	Description
EXP-file	<p>The EXP-file is a plain text file with information in the form of DATAPLOT Graphical Language commands. These commands can specify some or all of the data points in your POP-file. This allows you to plot these data points on top of your plotted optimization results (with the POST commands <a href="#">APPEND_EXPERIMENTAL_DATA</a> on page 192 or <a href="#">QUICK_EXPERIMENTAL_PLOT</a> on page 201). You can then visually assess the fit between these results and the experimental data. The PARROT workspace is not influenced in any way by the creation or use of EXP-files.</p> <p> Also see the <i>DATPLOT User Guide</i> included with this documentation set.</p>

## Optimization Workspaces

When writing the setup file, you enter a [CREATE\\_NEW\\_STORE\\_FILE](#) on page 94 command which creates a PARROT workspace file. Alternatively, select an existing PARROT workspace file with [SET\\_STORE\\_FILE](#) on page 116. The workspace file is automatically updated and saved with the latest optimization results (after each use of the [OPTIMIZE\\_VARIABLES](#) on page 109 command). You can also explicitly instruct Thermo-Calc to save the workspace using [SAVE\\_PARROT\\_WORKSPACES](#) on page 111. If you want to get rid of your latest changes and return to the state of your workspace when it was last saved, use [READ\\_PARROT\\_WORKSPACES](#) on page 109.

When the PARROT workspace is saved, parts of the POLY and GIBBS workspaces are also saved to the PARROT workspace file, along with the PARROT workspace itself. Using the POLY command [SAVE\\_WORKSPACES](#) on page 161 creates a new POLY3 file, nothing is saved to the PARROT workspace file.

If you do any POLY calculations based on data in the current workspace file, then a \*.POLY3 file is created, which contains a copy of the current set of parameters. If you continue on your optimization and read the old \*.POLY3 file, then the new set of parameters is overwritten with the old set. It is therefore recommended that you never read a \*.POLY3 or \*.GES5 file while you are doing an optimization.

## Method for Optimization and Simulation

The PARROT module typically uses ordinary POLY minimization for equilibrium calculations. The global minimization technique that is used in POLY cannot be used because it automatically creates new composition sets which corrupt the PARROT workspace. Furthermore, the equilibrium definitions that you use as input for your optimization must each be attributed to a specific phase. Some of these definitions may specify some local or partial equilibrium state rather than a global minimum. However, it is possible to use the global minimization technique for some equilibrium calculations by using the ED\_EXP command [ADVANCED\\_OPTIONS](#) on page 125 with the `Toggle_Alternate` option.

Optimization in PARROT is performed on the basis of a 'maximum likelihood' principle. According to this principle, the best fit between various calculated results and all the input of experimental data is found where the sum of the square of the weighted residuals is at its minimum.

Typically, the results of an optimization is considered to be better the fewer optimizing variables that are needed to get the same level of fit between computed results and experimental data. If you can get almost the same fit using eight instead of twelve parameters, then this should be considered to be a significant improvement. When more parameters are used, the values of the individual parameters tend to become unrealistic. This is particularly true when it comes to temperature-dependent parameters. However, relatively small differences in the number of parameters are often insignificant. For example, it does not typically matter whether you used 24 or 25 parameters to reach a certain degree of fit.

It is often difficult to compare the quality of different optimizations based on the number of optimizing variables that have been optimized. Since you may rely more or less heavily on different pieces of available experimental data (and do so with good reason), it is possible that two different users could end up with very different numbers of parameters for the same system. For example, suppose you optimize the Fe-Al system to incorporate it into an Al database, while someone else optimizes the same system to incorporate it into an Fe database. In this situation, the two of you would probably make different judgements about which experimental information your calculated results must have a good fit with.

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## Creating the POP-File

Before starting an optimization in Thermo-Calc, you must collect relevant experimental data about your system that is available in the research literature. This data is then entered in the POP-file. The experimental data points and measurements are entered in this plain text file in the form of ED\_EXP commands.

The syntax of the POP-file is in principle independent of the models used for describing the phases in the system.

In this section:

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<i>Experimental Information</i> .....	<i>13</i>
<i>POP-File Syntax</i> .....	<i>14</i>
<i>Entering Experimental Information</i> .....	<i>16</i>



## Experimental Information

An optimization of thermodynamic model parameters should be based on a range of reliable experimental results that is as wide as possible, as well as on empirical or semi-empirical correlations and theoretical considerations. During an optimization in Thermo-Calc, many kinds of thermochemical and thermophysical data can be mixed and used together.

The information needed for an optimization represent measurements of thermodynamic parameters in the system at equilibrium. These can be measurements of any of the thermodynamic quantities that can be set as conditions in Thermo-Calc. The information may represent measurements of activities or enthalpies in single-phase regions for example, or solubilities or transformation temperatures in a multi-phase region.

For each equilibrium that is used in the optimization, at least one quantity must have been measured and you also need to know the conditions that must be set to compute the system's equilibrium state. For example, consider a binary system in a single-phase region. Suppose that you have measured the temperature, pressure, composition and the chemical potential. Three of these quantities are necessary to specify the equilibrium state and the forth can be used as experimental information to model the phase.

If you have a two-phase region and know the temperature and pressure conditions, as well as which the stable phases are, then you could use the compositions of one or both phases as experimental data. The former information about the conditions is sufficient to determine the equilibrium. The experimental information can then be used to optimize the parameters that are used to characterise and model the system.



For examples how to enter various kinds of experimental data in the POP-file, see [Experiments and Experimental Data on page 50](#).

## Conflicting or Missing Information

You are likely to sometimes have inconsistent or conflicting experimental information. In principle, all available experimental data should still be entered into the POP-file, unless you have good reasons to exclude some information. For example, if you have reason to believe that the samples used in some experiments were not pure, then these experiments could be excluded from the POP-file.

For some systems, you have very little experimental data to go on. When this is the case, do not try to fit the available data uncritically with high accuracy without considering possible errors. You can look for data in systems with similar elements to get an idea about what the reasonable estimates of data that is lacking could be. Or you can use calculations from first principles or semi-empirical methods to get reasonable estimates that can be used as experimental data.

## Invariant Equilibria Information

The most valuable experimental information for an optimization is information about stable invariant equilibria. An invariant equilibrium is such that neither pressure, temperature nor composition can be changed without there being a change in the set of phases present in the system. It is recommended

that all information about invariant equilibria for a system is included in the POP-file. These equilibria need not all be based on explicit experimental measurements of thermodynamic properties.

Reasonable estimates from available experimental data are often useful to include in the POP-file. Such estimates, which should be based on the available experimental data, helps Thermo-Calc find a good set of start values on the optimization variables. However, at the end of the assessment, these estimated equilibria should be excluded and you should complete the optimization based only on the experimental information that is based on measurements.

With some experience from phase diagram evaluation, it is possible to make reasonable estimates of metastable invariant equilibria. Such estimates helps reduce the number of phases that are assessed simultaneously during the optimization. For example, you may assume that a certain intermediate phase does not form in a system. Then extrapolate the liquidus curves below the stable three-phase equilibria and finally, estimate temperatures and compositions of metastable three-phase equilibria between two other phases and the liquid.

Another useful technique is to extrapolate a liquidus line from a peritectic equilibrium to estimate the congruent melting temperature of a compound. This estimate may be more useful than the information about the peritectic equilibrium itself as the equilibrium involves only two phases.

### Equilibria in Higher-Order Systems Information

When you optimize a binary system, the available experimental information can often be described equally well by very different sets of parameters. Information about ternary and higher order systems that include the components of the binary system are then often useful for optimizing the binary system (the same is true of information about quaternary system with respect to optimizing ternary systems). Often, it is only when you extrapolate the optimized parameters to a higher-order system that you can judge which of the sets of model parameters that is best. Sometimes information from several ternary systems is required to make a reliable judgement about which set of parameters best describes a particular binary system.

### Heat Capacities Information

If you want to optimize your system based on data about heat capacities, then the corresponding parameters should first be optimized separately before you perform the general optimization of your system. The parameters should be kept fixed during the general optimization. This is because it is normally not possible to optimize heat capacity data together with other data in a meaningful way. If you do this, then it is very likely that the parameters related to the heat capacity are badly determined.

## POP-File Syntax

It is recommended that you specify an experimental equilibrium as close as possible to actual experimental conditions. Ideally, there is information about the set of stable phases, temperature, pressure and some or all compositions for the equilibrium.

In addition, it is recommended that you keep the POP-file well-organised and extensively commented. This is especially important if someone else reassesses the system when new experimental information is available.

If you have too many equilibria defined in your file, or if you define equilibria with different sets of components in the same file, then you must divide the POP-file in *blocks* (using the [FLUSH\\_BUFFER on page 41](#) command). You know whether you have defined too many equilibria for one block when you compile the file. A too large number of equilibria leads to an error message when the file is compiled.

If you use the [DEFINE\\_COMPONENTS on page 143](#) command, then it must be the first command in the POP-file (or if you have several blocks, DEFINE\_COMPONENTS can also be put as the first command after FLUSH\_BUFFER). This is because the command automatically reinitiates the current workspace, so the effect of any commands placed before it are not saved.



The last command in the POP-file should always be [SAVE\\_WORKSPACES on page 30](#).

### Legal Commands in a POP-File

The following commands can be used in a POP-file.



Also see the *Thermo-Calc Console Mode Command Reference Guide* for information about all these commands.

- [ADVANCED\\_OPTIONS on page 125](#)
- [CHANGE\\_STATUS on page 135](#)
- [COMMENT on page 40](#)
- [CREATE\\_NEW\\_EQUILIBRIUM on page 143](#)
- [DEFINE\\_COMPONENTS on page 143](#)
- [ENTER\\_SYMBOL on page 195](#)
- [EVALUATE\\_FUNCTIONS on page 155](#)
- [EXPERIMENT on page 24](#)
- [EXPORT on page 26](#)
- [FLUSH\\_BUFFER on page 41](#)
- [IMPORT on page 27](#)
- [LABEL\\_DATA on page 28](#)
- [SAVE\\_WORKSPACE on page 232](#)
- [SET\\_ALL\\_START\\_VALUES on page 162](#)
- [SET\\_ALTERNATE\\_CONDITION on page 30](#)
- [SET\\_CONDITION on page 165](#)
- [SET\\_NUMERICAL\\_LIMITS on page 168](#)

- [SET\\_REFERENCE\\_STATE](#) on page 169
- [SET\\_START\\_VALUE](#) on page 171
- [SET\\_WEIGHT](#) on page 33
- [TABLE\\_HEAD](#), [TABLE\\_VALUES](#) and [TABLE\\_END](#) on page 39

## Entering Experimental Information

A POP-file in Thermo-Calc (\*.POP) mainly consists of descriptions of equilibria, each equilibrium describing a data point that is based on an experiment from the existing literature on your system. An equilibrium is specified using ED\_EXP commands.

The following is an example of a specification of an equilibrium with a single stable phase in the Au-Cu system. Equilibria with a single stable phase are often from experiments where enthalpies of mixing or chemical potentials have been measured.

```
CREATE_NEW_EQUILIBRIUM 1 1
CHANGE_STATUS PHASE LIQUID=FIX 1
SET_CONDITION T=1379 P=1E5 X(LIQUID,AU)=0.0563
SET_REFERENCE_STATE AU LIQ * 1E5
SET_REFERENCE_STATE CU LIQ * 1E5
EXPERIMENT HMR=-1520:200
COMMENT Measurement by Topor and Kleppa, Met trans 1984
```

## Creating a New Equilibrium

The first command in an equilibrium specification is always [CREATE\\_NEW\\_EQUILIBRIUM](#) on page 143. This command takes two integers as arguments. The first integer should specify a unique identifier that can be used later to refer to the equilibrium in question. The second integer is an initialisation code 0, 1 or 2:

- Code 1: This means that all components are entered but all phases are suspended. This code is appropriate in most cases.
- Code 0: This means that all components and phases in the equilibrium are suspended initially. This code is needed if you are using experimental data about systems of different orders simultaneously, such as data about both binary and ternary systems for example.
- Code 2: This means that all components and phases are initially entered.

## Example

For example, the first command in the example above creates an equilibrium data point with the unique identifier 1. All components of the system are entered but all phases are suspended:

```
CREATE_NEW_EQUILIBRIUM 1 1
```

## Setting Equilibrium Conditions and its Uncertainty

All the equilibrium-related commands that are placed in between two [CREATE\\_NEW\\_EQUILIBRIUM](#) on [page 143](#) commands are interpreted as specifying the conditions of the equilibrium created by the first command. The values of these conditions should be based on the conditions specified in the experiment that you base the equilibrium definition on.

## Example

In the example, the [CHANGE\\_STATUS](#) on [page 59](#) command specifies that the equilibrium is a single-phase equilibrium with the liquid phase.

```
CHANGE_STATUS PHASE LIQUID=FIX 1
```

Furthermore, the temperature is 1379 K, the pressure is 1 bar (1E5 Pa) and the mole fraction of Au is 0.0563.

```
SET_CONDITION T=1379 P=1E5 X(LIQUID,AU)=0.0563
```

Sometimes you have reason to think that some information about an equilibrium condition may not be accurate. If this is the case, then you specify the degree of uncertainty for a condition with a colon after the condition quantity, directly followed by either an absolute value or a percentage. For example, if you have reason to doubt the reliability of the Au mole fraction measurement, then you could write:

```
SET_CONDITION T=1379 P=1E5 X(LIQUID,AU)=0.0563:10%
```

This indicates that you think the Au mole fraction is between 0.0507 and 0.0619. PARROT calculates the equilibrium twice, once for 0.0507 and once for 0.0619, and then computes the change of each experimental value between these two equilibria. This change is used to modify the uncertainty specified for the experimental value.



Also see [Entering the Experimental Value and its Uncertainty on the next page](#).

The possibility of specifying uncertainties on conditions may be useful when you have experimental data about a ternary system. In a binary system, a tie-line is determined by the two phases, the temperature and the pressure. Measurements of the compositions of both phases can then be used as experimental data. To specify the tie-line in a ternary two-phase equilibrium one of the four compositions must also be set as a condition. If the measurement of this composition has the same uncertainty as the other compositions, then you can assign this same degree of uncertainty both to the composition selected as a condition and the compositions selected as experimental data. Alternatively, the sample (overall) composition could be used as a condition and all four phase compositions could be used as experiment

values. These phases must have the status *entered* (not fixed) since the relative amount of each is unknown.

## Setting Reference States

If you want to specify a non-default reference state for one or several of your system components, then you do this with the [SET\\_REFERENCE\\_STATE on page 169](#) command. In the following example, the reference state for the liquid phase is set to current temperature (\*) and a pressure of 1E5 Pa.

### Example

```
SET_REFERENCE_STATE AU LIQ * 1E5
SET_REFERENCE_STATE CU LIQ * 1E5
```

Note that in order for these reference states to be taken into account when the measurement of the enthalpy per mole of the system is entered with experiment, the R-suffix must be used.

## Entering the Experimental Value and its Uncertainty

The [EXPERIMENT on page 24](#) command is used to specify the quantity that the calculated results should be fitted to. When specifying this quantity, you both specify the measured quantity itself and your estimation of the uncertainty of this value.

## Example

In the example, the EXPERIMENT command specifies the enthalpy per mole of the system, where this value is specified with respect to non-default reference states that you have set in the equilibrium specification:

```
EXPERIMENT HMR=-1520:200
```

The value before the colon is the quantity of the variable. The value after the colon is an assessment of the uncertainty of this quantity. A higher value means a greater uncertainty. In the example, the uncertainty has been specified with an absolute value but it could also be specified in percent of the quantity:

```
EXPERIMENT HMR=-1520:13%
```

Several experiments can be specified after the experiment command. Besides assigning values to conditions, it is also possible to specify that a certain quantity is greater than or less than a certain value. For instance, the following command would specify that the activity of the C-component is less than 0.01 and the mass fraction of the BCC phase of Ag is greater than 0.05:

```
EXPERIMENT ACR(C)<0.01:0.001 W(BCC,AG)>0.05:10%
```

Note that an experimental quantity can typically also be treated as an equilibrium condition, and vice versa. Which measured quantities that you treat as conditions and which quantities you treat as experimental data should be based on the accuracy of the different measurements. In most cases, the quantity that is based on the experimental technique with the lowest accuracy should be used as the experimental value.

## Entering Many Equilibria as a Table

When one thermodynamic variable (e.g. heat capacity) has been measured as a function of another (e.g. temperature), then experimental data is often presented as a table. By using the TABLE\_HEAD, TABLE\_VALUES and TABLE\_END commands, you can enter such experimental information into the POP-file in the form of a table. These three commands should always be used together and must be entered in the right order. See [TABLE\\_HEAD, TABLE\\_VALUES and TABLE\\_END on page 39](#).

The TABLE\_HEAD command is followed by a number. This number identifies the table as a whole, but also uniquely identifies the first equilibrium that is included in the table. This numeric identifier is incremented by one for each additional equilibrium in the table. Each row in the table represents one equilibrium. Thus, the equilibrium defined by the first row in the table above (on the line immediately below TABLE\_VALUE) is uniquely identified with the number 1, the equilibrium defined by the second row by number 2, and so on until the last equilibrium on the sixth row, which is identified by the number 6.

Since the unique identifiers of the equilibria in the table are automatically generated from the unique numerical identifier that you give to the table, the unique numerical identifier that is normally given to the [CREATE\\_NEW\\_EQUILIBRIUM on page 143](#) command is replaced by two at signs (@@).

At least one of the equilibria conditions specified with the [SET\\_CONDITION on page 165](#) command must be a condition whose value is set by the numbers in one of the table columns. To assign the numbers in a

column to a condition, use the syntax `SET_CONDITION <condition>=@<column number>`. For instance, in the example above, the mole fraction of  $X(\text{AlO}_3/2)$  is for each equilibrium given by the number in the first column of the table.

At least one of the measured variables that are entered with the experiment command must be a variable whose value is set by the numbers in a table column. To assign the numbers in a column to a measured variable, use the syntax `EXPERIMENT <variable>=@<column number>`. In the example above, the measured temperature for each equilibrium is given by the number in the second table column.

The actual table should be entered between `TABLE_VALUES` and `TABLE_END`. Separate the columns with tabs or any number of spaces. The columns do not have to contain numbers, but can also contain other types of values, such as phase names for example. If a column contains text with spaces or special characters, then the text must be surrounded by double quotes ("ABC DEF&ghi", for example). The table may have columns that are not used, but each row must have exactly the same number of columns.

### Example

The following block of commands exemplifies how a table can be entered into a POP-file:

```
TABLE_HEAD 1
CREATE_NEW_EQUILIBRIUM @@ 1
CHANGE_STATUS PHASE TETR=FIX 0
CHANGE_STATUS PHASE ION=ENT 1
SET_CONDITION P=101325 N=1 ACR(O2,GAS)=.21 X(AlO3/2)=@1
EXPERIMENT T=@2:5
TABLE_VALUE
0.46082476
0.57142380
0.66822276
0.7496 2176
0.50382426
0.63132249
TABLE_END
```

### Setting Site Fraction Start Values

In some systems, you have to set non-default composition start values on some experiments in order to get them to converge properly during optimization. This may be important if your system has a miscibility gap for example, in which case several equilibria with different compositions exist at certain temperatures. In such cases, you have to make sure it is specified in the POP-file which side of the



miscibility gap the equilibrium is on. The calculated equilibrium could otherwise end up on the wrong side, resulting in a large error.

In the POP-file, you can set the site fraction of a constituent on an equilibrium with [SET\\_START\\_VALUE](#) on [page 171](#).

### Example

For example, the following command sets the composition start value of VA constituent of the FCC\_A1 phase to 0.99:

```
SET_START_VALUE Y (FCC_A1, VA#2)=0.99
```

Setting the mole fraction for a component in a phase is not as reliable as setting the site fraction.

Additional equilibria entered after the last SET\_START\_VALUE command are automatically given a similar start value if the following command appears previously in the POP-file:

```
SET_ALL_START_VALUES Y
```

If start values are not set automatically for phase constituents, then you may have to set the composition start value for each equilibrium (or table of equilibria) separately.

## Commenting About an Equilibrium

The COMMENT command inserts a comment about the equilibrium that is saved to the PARROT workspace file when the POP-file is compiled. The comment must be entered on one line.

Comments can also be entered immediately after a dollar sign (\$), but these are not saved to the PARROT workspace. Instead, these comments are ignored by Thermo-Calc when the POP-file is compiled.

## Simultaneous Use of Binary and Ternary Experiments

You can use experimental information about binary and ternary systems (as well as systems of even higher order) in the same POP-file and optimization. To do this, you must inform the PARROT module that not all components of the ternary system (or system of even higher order) should be considered. This allows you, for example, to use experimental information about a binary equilibrium that exists within a ternary system.

Use [CHANGE\\_STATUS](#) on [page 59](#) with the keyword component and which components that should be entered. You should also give the initialization code 0 (rather than 1) to the [CREATE\\_NEW\\_EQUILIBRIUM](#) on [page 143](#) command. This code indicates that all components must be entered.

### Example

For example, the following set of ED\_EXP commands characterises a binary (A-B) three-phase equilibrium (FCC-BCC-LIQ) in a ternary system (A-B-C). It can be used in a POP-file that otherwise only contain experimental information about the ternary system (A-B-C):

```
CREATE_NEW_EQUILIBRIUM 1 0
CHANGE_STATUS COMPONENT A B = ENTERED
```

```
CHANGE_STATUS PHASE FCC BCC LIQ=FIX 1
SET_CONDITION P=1E5
EXPERIMENT T=1177:10
COMMENT from A-B
```

## Using Stability Conditions

Early in the optimization when parameter values are not so good it is often useful to set the driving force for precipitation of a phase (per mole of components) to make sure that it appears where it should. The DGM condition is very useful for making sure that phases appear where they should. It can be removed when the optimization becomes stable.

The DGM condition is also useful for suppressing phases that appear where they should not appear. Do this by setting the value and the uncertainty to something reasonable. For example, the driving force for precipitation of the BCC phase could be set as follows:

```
DGM(BCC) <-0.1:0.1
```

This produces an error even before BCC becomes stable and the weight of the experiment in question can be adjusted as needed. If you specify that the driving force for the BCC phase should be below 0 (DGM(BCC)<0:1E-4 for example), then the optimization converges extremely slowly (if at all). With such a sharp error condition, calculating the equilibrium is like finding the minimum point on a lawn that gently slopes towards a rock wall. The optimization keeps bouncing into the wall.

Another useful stability condition is the phase stability function, abbreviated QF. This can be used to specify that a phase is outside the miscibility gap for a solution phase. If QF(phase) is negative, then the phase is inside the miscibility gap; if QF(phase) is positive, then it is outside the miscibility gap.

## Grouping Equilibria with Labels

If you have several equilibria describing experiments that you want to be able to treat collectively, you can give all of the equilibria one and the same label.

Use LABEL to give an equilibrium a label. The label must start with the letter A and can only be up to four characters long. For example, you can insert the following command in several equilibria specifications:

```
LABEL ALH
```

During the optimization, you could use this label to, for example, set all the equilibria that have it to the same weight in the ED\_EXP module.

## Dividing the POP-File into Several Blocks

For two different reasons, you may have to divide your POP-file into different blocks:

- PARROT uses a buffer for storing compiled experimental data. If there is not enough memory in this buffer for storing all the experiments from the POP-file, then the POP-file can be divided into several blocks. When PARROT encounters the end of a POP-file

block, it saves the experimental data that has been compiled to PARROT workspace, clears out the memory buffer and then proceeds to read the next block in the POP-file. This goes on until the experimental data from all the blocks have been saved to the PARROT workspace.

- If you want to put equilibria with different sets of components in one and the same POP-file, then you must divide the file up into blocks. Each block should only contain equilibria that all have the same set of components.

To divide the equilibria in the POP-file into different blocks, enter the [FLUSH\\_BUFFER on page 41](#) command between two equilibria. This command marks the beginning of new block. When the command is encountered during the compilation of the POP-file, the compilation of the current block is terminated, the equilibria saved to the PARROT workspace file and a new block is initiated. That the buffer is reinitiated means that all functions and constants that were entered in the previous block must be entered again in new block in order to be used.

When editing your experimental data in the ED\_EXP module, you can select which block to load and edit using [READ\\_WORKSPACES on page 160](#) `<block number>`. The block before the first instance of FLUSH\_BUFFER is block number 1, the block after the first instance and before the second instance is block number 2, and so on.

---

## The Setup File

In this section:

---

<i>Creating the Setup File</i> .....	25
<i>Defining the System</i> .....	25
<i>Entering the Optimizing Variables</i> .....	26
<i>Initializing Optimizing Variables in PARROT</i> .....	28
<i>Creating the Workspace File</i> .....	29
<i>Compiling the POP-file</i> .....	29
<i>Returning Control to the Console</i> .....	29

---

## Creating the Setup File

The second step is to create the setup file. This is an ordinary Thermo-Calc macro file (\*.TCM). Typically, your setup file should contain the following:

- A system definition.
- A section where you enter model parameters and optimizing variables.
- A GO PARROT command.
- A section where initial values are assigned to the optimizing variables for the first optimization cycle.
- A [CREATE\\_NEW\\_STORE\\_FILE on page 94](#) <filename.par> which creates the PARROT workspace file onto which the results of your optimization are continuously saved and updated. By default this workspace file has the same filename as the setup file, but with the \*.PAR filename extension.
- A [COMPILE\\_EXPERIMENTS on page 92](#) <filename.pop> command. Since you often encounter syntax errors when you first try to compile a POP-file, it may be useful to execute this command from the console rather than as part of the setup macro file.
- Normally, you also have a [SET\\_INTERACTIVE on page 8](#) at the end of the setup file. This command returns control over Thermo-Calc to the console.

It is possible to interactively execute all these commands one at a time in the console. It may be instructive to enter the commands that would normally go into the setup file interactively while using the on-line help while you are learning to use the PARROT module.

## Defining the System

If you have an existing database with information about your system, then you can write the system definition part of your setup file in two different ways.

- If you have an unencrypted user database, then you can define your system by entering DATA module commands directly in the setup file. Use the DATA commands that you normally use to define a system when doing equilibrium calculations in Thermo-Calc Console Mode.
- Define your system by entering DATA module commands directly in the console, then generate a macro file with the GIBBS command [LIST\\_DATA on page 77](#) <name of setup file>.tcm p . This command saves all the data that has been loaded in the GIBBS workspace as a macro file. This file can then be modified as required into an optimization setup file.

## Creating Additional Composition Sets of a Phase

If you need several composition sets of a phase, then these should be created with the GIBBS command [AMEND\\_PHASE\\_DESCRIPTION on page 52](#) `<phase name> composition_sets <composition set number>` in the setup file.



If you add composition sets of a phase after the POP-file has been compiled, the data structure in the workspace is corrupted and you have to recompile the POP-file.

## Entering the Optimizing Variables

When you have retrieved the data about your system for the setup file, you must manually enter the model parameters that you want to optimize. This is done using the GIBBS command [ENTER\\_PARAMETER on page 99](#), but when you specify the Gibbs energy expression for the parameter, you enter variables that can be given various values into the expression. It is the values of these variables (and thus, the Gibbs energy of the parameter) that you are optimizing.

How you in detail specify the optimizing variables in your set up file depends on which phase you are trying to optimize and what thermodynamic model that is used in the optimization.



Also see [Thermodynamic Models on page 59](#) for a range of examples.

## Entering Optimizing Variables in Parameter Specifications

There are ninety-nine predefined variables in the PARROT module which you can use in your optimization. These variables are referred to as `V1`, `V2`, `V3`, ... `V98` and `V 99`. When the GIBBS workspace is initialised, all optimizing variables are set to a fixed numerical value of zero. When you do an optimization, there is always some variable for which you want to evaluate the best value, but you can assign fixed values to optimizing variables too. It is often useful to enter all the variables that you can conceivably want to optimize, and then you can interactively select and change which variable to focus at various stages of the optimization.

The setup file excerpts that follow show how optimizing variables are entered. However, before the optimizing variables are introduced in this example, the following command enters an ionic liquid solution phase (a phase for which you have some experimental information):

```
ENTER_PHASE IONIC_LIQ Y,  
AL+3,ZR+4 ; ALO2-1,O-2 ; N N
```

This [ENTER\\_PHASE on page 69](#) command enters a phase called IONIC\_LIQ into the GIBBS workspace. This phase is of the type ionic liquid solution, which is specified by type code `Y`. Such a phase is modelled by the *Ionic Two Sublattice Liquid Model*. The next two arguments specify the two sublattices, in this case the cations `AL+3,ZR+4` and the anions `ALO2-1,O-2`. Components that interact in a sublattice are separated by a comma. The first `N` at the end means that no additional constituents are added to the phase. The second `N` means that a list of possible parameters for the phase should not be shown in the console.

There are model parameters that describe the phase which you do not want to optimize, in which case the Gibbs energy expression of the parameter does not contain any optimizing variables.

### Example 1

For example, the following parameters of the IONIC\_LIQ phase do not contain any optimizing variables:

```
ENTER_PARAMETER G(IONIC_LIQ,AL+3:ALO2-1;0) 298.15 +2*GAL2O3_L; 6000 N
ENTER_PARAMETER G(IONIC_LIQ,AL+3:O-2;0) 298.15 +GAL2O3_L+400000; 6000
N
ENTER_PARAMETER G(IONIC_LIQ,ZR+4:O-2;0) 298.15 +2*GZRO2L; 6000 N
```

These parameters define the Gibbs energy expressions for three constituents in the constituent array, namely AL+3:ALO2-1, AL+3:O-2 and ZR+4:O-2. The names that occur in these expressions—that is, GAL2O3\_L and GZRO2L—are the names of complex functions of temperature that are entered in the GIBBS workspace with the [ENTER\\_SYMBOL on page 72](#) command.

The numbers that frame the Gibbs energy expressions specify the temperature range within which the expression should be applied. In the above, the expressions are applied in a temperature range from 298.15 K to 6000 K.

### Example 2

In this example, suppose that you want to optimize the model parameter for the ZR+4:ALO2-1 combination, then you could enter the variables V1 and V2 in the Gibbs energy expression for that parameter in the following way:

```
ENTER_PARAMETER G(IONIC_LIQ,ZR+4:ALO2-1;0) 298.15 +GZRO2L +2*GAL2O3_L
+V1+V2*T; 6000 N
```

You normally have different optimizing variables in different parameters, but in some cases you may want several parameters to vary together, in which case you can use the same variable in the Gibbs energy expressions of several parameters.

## Entering Interaction Parameters

For some systems, you have to consider interaction parameters in order to take excess Gibbs energy into account and correctly model the phase. By default, the software uses a Redlich-Kister expression for the excess Gibbs energy. The coefficient is entered after the constituent array when you use the [ENTER\\_PARAMETER on page 99](#) command. In the last section, all the parameters were entered with a coefficient of zero (0).

### Example

To take account of the excess Gibbs energy, you might enter the following:

```
ENTER_PARAMETER L(IONIC_LIQ,ZR+4:ALO2-1,O-2;0) 298.15 +V11+V12*T;
6000 N
```

```

ENTER_PARAMETER L(IONIC_LIQ,ZR+4:AL02-1,O-2;1) 298.15 +V13+V14*T;
6000 N

ENTER_PARAMETER L(IONIC_LIQ,ZR+4:AL02-1,O-2;2) 298.15 +V15+V16*T;
6000 N

```

Parameters with interaction coefficients are referred to as *interaction parameters*. The regular parameter has a coefficient of 0. The subregular parameter has a coefficient of 1. It is possible to interaction coefficients up to a value of 9, but you are advised not to use more than three coefficients (that is, with coefficient values of 0, 1 and 2).

## Initializing Optimizing Variables in PARROT

Variables that have been entered into Gibbs energy expressions for model parameters in the setup file has to be initialized and given start values before they are optimized.

You have to estimate what start values to give to the optimizing variables based on your knowledge of the system or of relevantly similar systems. There are no general rules for what start values your optimizing variables should have. If you are not able to make any informed estimation about what start values to use, then you may not be able to find a good fit between your experimental data and your calculated results. In this case, it is often best to start the optimization in the so-called alternate mode. In alternate mode, the PARROT module helps you find some reasonable start values for your optimizing variables.



Also see [About Alternate Mode on page 43](#).

Even if you are starting your optimization in alternate mode, you still have to initialize the optimizing variables though (you can all give them a start value of 0).

To initialize an optimizing variable and to give it a start value, use either [SET\\_OPTIMIZING\\_VARIABLE on page 114](#) or [SET\\_SCALED\\_VARIABLE on page 115](#). Using SET-OPTIMIZING\_VARIABLE results in a scaling factor equal to the current value of the parameter unless the current value is zero, in which case the scaling factor is 1000. This is typically appropriate for enthalpic parameters, but not necessarily for other parameters. The scaling factor is the factor by which the optimizing variable value is varied during the optimization.

### Example

For example, if you want to optimize the variables V1, V2, V11, V13 and V17, then you could enter the following in the setup file:

```

SET_OPTIMIZING_VARIABLE 1 +43000
SET_OPTIMIZING_VARIABLE 2 -35.2
SET_OPTIMIZING_VARIABLE 11 +72000
SET_OPTIMIZING_VARIABLE 13 +27000
SET_OPTIMIZING_VARIABLE 17 -100000

```



The value given to each optimizing variable (+43000 for variable V1 for example) is also that variable's initial scaling factor. If you want to set the initial scaling factor of a variable to a value that is lower or higher than its start value, then use `SET-SCALED_VARIABLE <start value><scaling factor><min value><max value>`.

## Creating the Workspace File

In the setup file, after the system definition and the entered optimizing variables, use the PARROT command `CREATE_NEW_STORE_FILE` on page 94 to create and save a PARROT workspace file for the system defined in the setup file. For example, the following command saves all current data on system definitions (elements, species, components, phases), symbol definitions (constants, variables, functions, tables) and parameters that are stored in the workspace used by GIBBS, POLY and PARROT into a file called AL2O3-ZRO2.PAR:

```
CREATE_NEW_STORE_FILE AL2O3-ZRO2
```



The experimental information in the POP-file is not saved to this PARROT workspace file.

## Compiling the POP-file

At the end of the setup file, use the command `COMPILE_EXPERIMENTS` on page 92 followed by the name of your POP-file to compile the data in that file and save it to the current PARROT workspace file. Note that you must first have opened or created a new PARROT workspace file before you compile your POP-file. The other argument to the command can typically be given default values with comma signs (,):

```
COMPILE_EXPERIMENTS AL2O3-ZRO2.POP,,,
```

If Thermo-Calc encounters errors in the syntax of the POP-file, then error messages are displayed in the console. Normally, the compilation also stops when syntax errors are encountered. If this happens, then you must correct the errors and recompile the file. It is useful to have two console windows open when you do this. That way, you can use one console for editing the experimental data and another console for compiling and reading any further error messages.

## Returning Control to the Console

Put the command `SET_INTERACTIVE` on page 8 at the end of the setup file if you want to return control to the console when the commands in the setup file have all been executed.

---

## Optimizing in PARROT

In this section:

---

<i>Optimizing the System in PARROT</i>	<i>31</i>
<i>Changes that Require POP-file Recompilation</i>	<i>31</i>
<i>Optimization Workflow</i>	<i>31</i>
<i>Ensuring Computation of all Equilibria</i>	<i>32</i>
<i>Setting Weights</i>	<i>33</i>
<i>Optimizing and Evaluating Results</i>	<i>34</i>
<i>Continuing the Optimization and Resetting Variables</i>	<i>35</i>
<i>Updating the Set of Optimizing Variables</i>	<i>36</i>
<i>Reducing the Number of Optimizing Variables</i>	<i>38</i>
<i>Plotting Intermediate Results</i>	<i>38</i>

## Optimizing the System in PARROT

When you have created a POP-file, a setup macro file and (optionally) EXP-files, you should start doing optimization runs interactively in the console. This process can be divided into a number of steps (such as running optimization, evaluating optimization results, modifying weights and models and adding new information), but usually, you have to go through many optimization cycles before achieving a satisfactory fit between calculation results and experimental data.

Typically, it is not obvious when an optimization is finished. You must exercise your judgement about when the fit you have achieved is good enough.



It is possible to interactively change almost everything in the initial setup macro file and in the POP-file. For example, you can add more parameters to be optimized and modify or add more experimental information.

## Changes that Require POP-file Recompilation

Some changes that you do interactively in the PARROT module or the ED\_EXP sub-module destroys the data structure in the workspace. For example, if you add more composition sets to a phase, then the number of phases actually change and the links break between the experimental data and the thermodynamic models. Note that if the global minimization technique is used in POLY, then new composition sets that corrupts the PARROT workspace may be created automatically. If this happens, then you have to compile the POP-file again.

If you recompile the POP-file, then the experimental equilibria are calculated with the default start values.

## Optimization Workflow

Normally, the workflow during an optimization is the following:

1. In the PARROT module, run the setup macro file using [MACRO\\_FILE\\_OPEN](#) on page 5.
2. Go to ED\_EXP with [EDIT\\_EXPERIMENTS](#) on page 95, use [READ\\_WORKSPACES](#) on page 160 to load your experimental data and then execute [COMPUTE\\_ALL\\_EQUILIBRIA](#) on page 23.
3. If an equilibrium cannot be computed, then this either means that the start values (site fractions, for example) were inappropriate or that the equilibrium cannot be calculated with the current set of parameters. If the latter, then the equilibrium may have to be excluded from the optimization. However, you should make an effort to exclude the possibility that the reason is just that you do not have the appropriate start values for the equilibrium.
4. When each equilibrium is either successfully computed or excluded from the calculation, go back to the PARROT module and run the [OPTIMIZE\\_VARIABLES](#) on page 109 command. Give the number of optimization iterations you want the Thermo-Calc

program to carry out as an argument to the command. This number specifies how many different sets of values for the optimizing variables that PARROT tries to fit with the experimental data. It is recommended that you run 0 iterations first to see the discrepancy between the experimental data and the initial calculated results. The current workspace file is automatically updated with the last set of optimized variables and calculated results.

5. List and evaluate the result of the optimization using [LIST\\_RESULT on page 104](#). Typically, what is of interest in the results are the relative standard deviation of the optimizing variables and the error values in the list of calculated experimental data results. If the relative standard deviation for an optimizing variable is very large, this means that the variable doesn't have any effect on the computed results and that the variable should not be used (you can make PARROT ignore the variable by setting its value to 0 with [SET\\_FIX\\_VARIABLE on page 112](#)). If the relative standard deviation is close to zero for a variable, then this might indicate that you need to use more variables. When it comes to errors in the calculated equilibrium results, these can be decreased by lowering the weight that PARROT gives the experiment in the calculation (the more weight, the more the experiment affects the calculated results).
6. Use [OPTIMIZE\\_VARIABLES on page 109](#) or [CONTINUE\\_OPTIMIZATION on page 94](#) to carry out a new optimization cycle. Go back to step 5 above and continue to do optimization cycles until you judge that there is a good enough fit between your calculated results and your experimental data. It is recommended that you do not only rely on feedback from [LIST\\_RESULT on page 104](#) but also frequently plot various diagrams and compare them visually to some of your experimental data.

## Ensuring Computation of all Equilibria

When you have run the setup macro file, you should start by trying to compute all the equilibria that were created when your POP-file was compiled. To do this, you must first go to the ED\_EXP submodule, and load the experimental data from the current PARROT workspace file with the [READ\\_WORKSPACES on page 160](#) `<block #>` command (normally, the block number is 1).

When you have loaded all equilibria, you should try to compute them all using the ED\_EXP command [COMPUTE\\_ALL\\_EQUILIBRIA on page 23](#). A list of calculated equilibrium results are shown in the console, but the software is not able to reach an equilibrium for an experiment, then the program cancels the calculations and displays an error message.

The following list shows an example output where the first two experiments in the POP-file have been successfully computed, but an equilibrium is not reached for the third experiment. No other equilibria are computed, since the calculations are aborted when the error occurs.

Eq	Lab	Iter	Weight	Temp	Exp	Fix	phases	or	comments
1	A1	22	1.	2575.3		IONIC_	FLUORI	TETR	
2	A1	18	1.	2156.9		IONIC_	CORUND	TETR	

```
*** ERROR 1614 IN QTHISS
*** CONDITIONS CAN NOT BE FULLFILLED
```

When this happens, try to find out why the equilibrium calculation fail. Are the condition start values that you have given the equilibrium inappropriate for example? If you have a similar equilibrium that has already been successfully computed, then you can select the equilibrium that does not work, use the ED\_EXP command [SET\\_ALL\\_START\\_VALUES on page 162](#) and accept all the suggestions for the site fractions. Alternatively, use [TRANSFER\\_START\\_VALUE on page 34](#)<equilibrium number> to make the currently selected equilibrium inherit the start values of the indicated equilibrium. Run [COMPUTE\\_EQILIBRIUM on page 139](#) again to see if the equilibrium can be computed with the inherited start value.

If you cannot find an explanation of why the equilibrium cannot be computed, then it may be that the experiment is faulty. If so, then this experiment should be excluded from the optimization by being given a weight of 0. You should then run [COMPUTE\\_EQILIBRIUM](#) again to make sure that all equilibria can be computed. However, experiments that fail to reach equilibria could succeed in doing so if the optimizing variables have other values. It is therefore sometimes worth trying to include experiments later in the optimization process (when the optimizing variables are relatively close to their final values), even if they had to be excluded at its start. In some cases, it might also be appropriate to change the error tolerance for in an experiment (using the ED\_EXP command [EXPERIMENT on page 24](#)).



You must save the PARROT workspace with [SAVE\\_WORKSPACES on page 30](#) before you exit the ED\_EXP module.

## Setting Weights

To change the weight of an experiment, first enter the ED\_EXP module from PARROT using [EDIT\\_EXPERIMENTS on page 95](#). Then use the [SET\\_WEIGHT on page 33](#) command to set the weight for a specific equilibrium (equilibrium number 3 for example), for a range of equilibria (the equilibria 10–19) or all the equilibria that have a certain label (such as all the equilibria with the label A1). To save the new weight(s), use [SAVE\\_WORKSPACES on page 30](#).

By default, all the experimental information in your POP-file is treated equally: each experiment has a weight of 1. However, experiments that you excluded because they did not reach equilibrium now have a weight of 0. The higher the weight of an experiment is, the more Thermo-Calc tries to ensure that the computed result fits the condition measured in that experiment.

The contribution of an experiment's error to the sum of errors is multiplied by the square of the weight set for that experiment. In other words, if you want to cut the error of an experiment with weight 1.0 by half, then you should use a weight of 0.7. This makes the experiment's error 0.49. Setting the weight to 1.4 instead makes the error twice as large (1.96).

Note that if you use [READ\\_WORKSPACES on page 160](#) after you have changed weights on the experiments, your changes are lost unless you have saved those changes. In the ED\_EXP module, you can get a list of all the experiments in the console if you first read the experimental data from the workspace file (with [READ\\_WORKSPACES](#)) and then use [LIST\\_ALL\\_EQILIBRIA on page 28](#).

## Optimizing and Evaluating Results

When you have ensured that all the experimental data points can reach equilibrium, go back to the PARROT module and use `OPTIMIZE_VARIABLES` on page 109 <number of iterations> with 0 iterations. Present the result of this initial optimization by using `LIST_RESULT` on page 104.

When evaluating the optimization results, the most important information is found in the list of experiments at the end of the listed results. The rightmost column shows the difference between the value of the experimental data and the value computed by Thermo-Calc in the last optimization cycle.

The following shows part of list of experiments in the output of a `LIST_RESULT` command:

106 ACR(B)=0.34	0.3127	2.89E-02	-2.7282E-02	-0.9444	
107 ACR(B)=0.23	0.2085	2.89E-02	-2.1522E-02	0.7450	
108 ACR(B)=0.12	0.1042	2.89E-02	-1.5761E-02	-0.5455	
110 HMR(LIQUID)=-1964	3.6380E-12	5.00E+02	1964.	3.928	
111 HMR(LIQUID)=-3500	0.000	5.00E+02	3500.	7.000	*
112 HMR(LIQUID)=-4588	0.000	5.00E+02	4588.	9.176	*
113 HMR(LIQUID)=-5239	7.2760E-12	5.00E+02	5239.	10.48	*
114 HMR(LIQUID)=-5454	-3.6380E-12	5.00E+02	5454.	10.91	*
115 HMR(LIQUID)=-5233	1.8190E-12	5.00E+02	5233.	10.47	*
116 HMR(LIQUID)=-4575	-1.8190E-12	5.00E+02	4575.	9.150	*
117 HMR(LIQUID)=-3481	-1.8190E-12	5.00E+02	3481.	6.962	*
118 HMR(LIQUID)=-1950	0.000	5.00E+02	1950.	3.900	

PARROT:

The experiments for which the optimization has not found a good fit are marked with an asterisk (\*) or a hash sign (#) in the rightmost column. An asterisk in this column indicates that the experiment has an error that is larger than the error tolerance and a hash sign indicates that the error is much larger. The error tolerance depends on the degree of accuracy set for that particular piece of experimental information. The error values are presented in the next to rightmost column.

Note that if you are optimizing in *alternate mode*, then you usually do not need to change the weights for the experiments. Instead, you can simply run `OPTIMIZE_VARIABLES` again, specifying, say, thirty iterations, evaluate the results again, and continue in that way until you are satisfied with the results.



Also see [About Alternate Mode](#) on page 43.

## The Critical Set of Experiments

The set of weighted experiments that you end up with as a result of your optimization is referred to as the *critical set* of experiments. When you work to determine this set and the weights of the experiments, the following factors should be reflected in both the selection of experiments and the weights of those experiments:

- The reliability of the experimental technique.
- The extent of agreement/disagreement between independent measurements of the same quantity.
- The extent of agreement/disagreement between data obtained with different experimental methods.

## Continuing the Optimization and Resetting Variables

To continue the optimization after you have used *OPTIMIZE\_VARIABLES* on page 109, you can either use this command and enter <Number of iterations> again or *CONTINUE\_OPTIMIZATION* on page 94 <Number of iterations>.

If you use *CONTINUE\_OPTIMIZATION* on page 94, then PARROT continues the optimization using the same Hessian matrix. If the optimization is going well but you run out of iterations, then continuing with the same Hessian matrix may be useful.

As before, use *LIST\_RESULT* on page 104 to inspect the fit between the calculated and the experimental values for your experiments. If necessary, adjust the weights of the experiments again in the ED\_EXP module. You may even discover that you have to exclude additional experiments from the optimization.

Besides looking at the rightmost column in the list of experiments (that is produced when you use *LIST\_RESULT*), it is also useful to look at the *sum of squares* of the errors of all the variables. This is shown in the output of *OPTIMIZE\_VARIABLES* and *CONTINUE\_OPTIMIZATION*. This sum should be as low as possible.

### Example Output

The following shows part of the output that you get when using *LIST\_RESULT* on page 104:

```
== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.   VALUE           START VALUE   SCALING FACTOR   REL.STAND.DEV
V1      6.94641846E+05    4.30000000E+04    4.30000000E+04    1.42299558E+00
V2     -3.32619842E+02   -3.52000000E+01   -3.52000000E+01    7.91369573E-01
V11     8.37422071E+04    7.20000000E+04    7.20000000E+04    2.02212692E-01
V13     2.65253341E+04    2.70000000E+04    2.70000000E+04    1.45201828E-01
V17    -3.66637428E+05   -1.00000000E+05   -1.00000000E+05    8.04279315E-01

NUMBER OF OPTIMIZING VARIABLES :    5
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM    3.50196879E+05 TO    3.49096720E+05
DEGREES OF FREEDOM    14.  REDUCED SUM OF SQUARES    2.49354800E+04
```

In the example you can see that the sum of squares have decreased slightly. (The final sum of squares that you get after an optimization run is also presented directly in the output from *OPTIMIZE\_VARIABLES* and *CONTINUE\_OPTIMIZATION*.) As long as the sum of squares figure is decreasing, the optimization is working as it should.

When your calculated results have been improving for a while, that is, when the sum of squares has been decreasing, and you are confident that you are making definitive progress, then you should use the PARROT command [RESCALE\\_VARIABLES on page 110](#) to reset the starting values of the optimizing variables to their current values. When you do this, the start values and scaling factors of the optimizing variables (shown in the table's third column in the preceding screen shot), are all set to the current values (shown in the table's second column).

If your optimization is not going well, then you may want to reset the values of your optimization variables to their current start values. To do this, use [RECOVER\\_VARIABLES on page 110](#).

After rescaling the variables, continue the optimization using OPTIMIZE\_VARIABLES again. Cycle through calls of the commands OPTIMIZE\_VARIABLES/CONTINUE\_OPTIMIZATION, CONTINUE\_OPTIMIZATION, RESCALE\_VARIABLES and OPTIMIZE\_VARIABLES again until your set of optimizing variables does not seem to improve anymore. Even when it seems to you that you have reached this point, it is recommended that you use OPTIMIZE\_VARIABLES/CONTINUE\_OPTIMIZATION a few extra times to make sure that the variable values cannot be further improved, that is, that the sum of squares of the errors of all the variables cannot be reduced further. If the final solution is repeatedly calculated after the same number of iterations and reaching the same result, then it is generally reasonable to accept the current variable values.

## Updating the Set of Optimizing Variables

Besides evaluating the fit between the calculated results and the experimental data, you should also ensure that you have the right number of optimizing variables. If you have too many or too few optimizing variables, then you may not be able to use your model to accurately extrapolate thermodynamic properties in a wide range of temperature, pressure and composition conditions.

With more optimization parameters, the sum of errors usually decrease, but the parameters also tend to become less precisely determined. A measure of this precision is the Relative Standard Deviation (RSD) of each optimizing variable. However, the RSD is only significant if you have used [RESCALE\\_VARIABLES on page 110](#) followed by an optimization which converges and the values of the variables do not change much. The RSD tells you how much the parameter can be changed in either a positive or in a negative direction without changing the reduced sum of errors with more than one unit.

### Example

A large RSD value thus means that the parameter has not been determined well.



== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.01820948E+04	2.01874462E+04	2.01874462E+04	2.60519742E-02
V2	-2.90936164E+01	-2.90969472E+01	-2.90969472E+01	1.41576516E-02
V11	-2.18127453E+04			
V12	1.55559524E+01			
V15	2.36701148E+04	2.37258719E+04	2.37258719E+04	1.00528931E-01
V16	-7.56541897E+00	-7.64417807E+00	-7.64417807E+00	3.17218507E-01
V17	3.00342429E+03	3.02274918E+03	3.02274918E+03	2.60675550E-01
V19	2.20133190E+04	2.14534347E+04	2.14534347E+04	6.92923849E-01
V20	-6.72498276E+00	-6.31334932E+00	-6.31334932E+00	1.79242248E+00

NUMBER OF OPTIMIZING VARIABLES : 7

ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO

THE SUM OF SQUARES HAS CHANGED FROM 1.51360340E-01 TO 1.44420287E-01

DEGREES OF FREEDOM 18. REDUCED SUM OF SQUARES 8.02334928E-03

If such a significant RSD has a value larger than 1, then this typically means that you are using too many optimizing variables. However, the RSD values also depend on the weighting of the experiments, so it is sometimes possible to reduce the RSD by changing weights.

The RSD should not be too low either. If one or more of them is very close to 0, then this suggests that you are trying to optimize the system with too few optimizing variables. You can add optimizing variables interactively using [ENTER\\_PARAMETER](#) on page 99 in GIBBS. However, it is recommended that you add a sufficient number of variables in the setup file from the start so that do not need to do this. You can fix variables to a value of 0 until you discover that they are needed.

Besides the RSD, you should also keep an eye on the variable values themselves (shown in the VALUE column, next to the leftmost column in the table shown in the preceding screenshot). If the value of a variable is in the order of 1E5 or higher and this variable has been put in the temperature-independent part of an interaction parameter's Gibbs energy expression, then you may not have the right weights on your experiments or you are using too many optimizing variables. This is also typically the case if a variable with a value in the order of 10 or more (per mole atoms) is in the temperature-dependent part of the Gibbs energy expression of an interaction parameter. Such a high parameter value may lead to inverted miscibility gaps or re-stabilisation of a phase at high temperature. It is important to keep an eye on this since the temperature-independent and the temperature-dependent interaction parameter often varies together. If the temperature-dependent interaction parameter cannot be reliably determined, you may have to fix its value.

Note that even if you have found a good enough fit between calculated and experimental values after an optimization run, a parameter value may suddenly start to change by several orders of magnitude when you use [OPTIMIZE\\_VARIABLES](#) on page 109 is used again. If this happens, then careful reconsideration of the weighting of the experiments of the set of optimizing variables is required. However, when the optimization has converged and the parameter values remain stable after repeated use of OPTIMIZE\_VARIABLES, this should usually not happen.

## Reducing the Number of Optimizing Variables

If you have one or more optimizing variables with RSD larger than 1, then you should remove one or more of the variables by setting them to a value of 0, or alternately, set them to a reliably estimated value (estimated based on, for example, semi-empirical methods).

To fix an optimizing variable to certain value, use the PARROT command [SET\\_FIX\\_VARIABLE on page 112](#)  
<variable number> <value>.

## Plotting Intermediate Results

It is typically not sufficient to look at the plain text output of [LIST\\_RESULT on page 104](#) to reliably judge how the optimization is progressing. Plotting a phase or property diagram of the system you are optimizing using the POLY and POST modules is often very useful.

It is recommended that you create a macro file for plotting the diagram since you probably want to repeatedly plot the diagram as you progress with the optimization. This macro file can then be called directly from the PARROT module with the [MACRO\\_FILE\\_OPEN on page 5](#) command.

## Superimposing Experimental Data from EXP-files

If you create one or several EXP-files based on the experiments in your POP-file, you can visually compare the fit your plot and the experimental data you are optimizing the system against. An EXP-file contains data points specified in the DATAPLOT format. You could make an EXP-file for each type of data that you are using in the optimization.

Use the POST command [APPEND\\_EXPERIMENTAL\\_DATA on page 192](#) to superimpose the data points in an EXP-file on a phase or property diagram that you have plotted. For example, to put the experimental data points from a file entitled DP.EXP onto a plotted diagram, you could enter the following:

```
APPEND_EXPERIMENTAL_DATA Y DP.EXP 0 1
```

Such a command call tells Thermo-Calc to superimpose the data points in dataset 1 of DP.EXP onto the plot in the Console Results window, but not to impose any information about axis scaling, labels and other information which is normally found in the prologue of the DP.EXP file.

The POST command [QUICK\\_EXPERIMENTAL\\_PLOT on page 201](#) can also be used to superimpose data points on a plotted phase or property diagram.



Also see the *DATPLOT User Guide* included with this documentation set.

---

## Finalizing the Optimization

In this section:

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<i>Finishing the Optimization</i> .....	<a href="#">40</a>
<i>Rounding off Optimizing Variable Values</i> .....	<a href="#">40</a>
<i>Updating the Database File</i> .....	<a href="#">40</a>
<i>Creating a Database File</i> .....	<a href="#">41</a>
<i>Updating the Setup File and the POP-file</i> .....	<a href="#">41</a>

## Finishing the Optimization

When to stop optimizing is a matter of judgement. It is rarely the case that you finish optimizing a system with the feeling that it cannot be improved.

The final step is to update your files with the final results. Besides updating your database file (or alternatively, creating a new database file), it is advised that you also update your setup and POP-files with the final weights and optimizing variable values.

## Rounding off Optimizing Variable Values

When you save the optimizing variable values, it is important that you round off the values correctly. When you have a metallic system, it is usually best to keep whatever number of decimal digits that you need to make less than one J/mol difference at 1000 K. When you have an aqueous system or a system that you are optimizing based on data from very different temperature ranges, then this is not always the only appropriate guideline. However, rounding off the values in such a way that it gives a difference that is larger than one J/mol may lead to differences in the phase diagram.

Another approach you can take when rounding off variable values is by progressively fixing the value of more and more of the variables. This allows you to round-off all but one of the variables values so that each only has a few significant digits. Variables whose values have been rounded off in this way are easier to handle compared with those that are rounded off so that they continue to have many significant (non-zero) digits.

To round off the variable values according to this second approach, first use [SET\\_FIX\\_VARIABLE on page 112](#) to set the variable(s) with the highest RSD to a rounded off value (such as, say, 0.4). When you then re-optimize using [OPTIMIZE\\_VARIABLES on page 109](#), the sum of errors changes. However, you should get almost exactly the same sum of errors as before after you rescale the variable values using [RESCALE\\_VARIABLES on page 110](#). (If the sum of errors is different, then this means that the variable with the highest RSD was not rounded off in a good way.) If you successfully round off the first variable value, then continue to round off the optimizing variable which now has the highest RSD. Continue doing this until you have fixed all but one of the optimizing variables to their rounded-off values. The final sum of errors that you get after having fixed the variable values should not deviate significantly from the initial sum of errors you had before starting to round-off the variable values.

## Updating the Database File

To update the database file (with filename extension TDB) open it in a text editor and enter or update each of the parameters that you have optimized.

For example, suppose you have the following command in your setup file:

```
ENTER_PARAMETER L(IONIC_LIQ,AL+3,ZR+4:O-2;0) 298.15 +V17; 6000 N
```

If you then end up with a value for optimizing variable V17 of -100000, then you should enter the following under the IONIC\_LIQ phase in the database file:

```
PARAM L(IONIC_LIQ,AL+3,ZR+4:O-2;0) 298.15 -100000; 6000 N REF !
```



If you often need to round-off the optimizing variable value in some way, see [Rounding off Optimizing Variable Values](#) on the previous page.

When you have updated or entered the parameters that you optimized, save the database file.

## Creating a Database File

In some circumstances you may want to save all the information about your system into a new database file. To do this, go to the GIBBS module and use `LIST_DATA <Filename> N`. This creates a new user database file that contains all the information about the system that is in the workspace.

The N-argument tells the [LIST\\_DATA on page 77](#) command to save the output into database file rather than some other type of file, such as a macro file for example. Note that the output database file that you get from `LIST_DATA` have to undergo some manual editing before it can be used as proper database file.

## Updating the Setup File and the POP-file

It may be useful for you to be able to recreate your optimization from scratch. It is therefore recommended that you do the following when you are done with the optimization:

- Update your POP-file so that it contains the weights of your critical set of experiments. Use [SET\\_WEIGHT on page 33](#) to set the weights directly in the POP-file. You may also have to use [SET\\_START\\_VALUE on page 171](#) for some conditions in the POP-file. Otherwise, you may not be able to compute the equilibria with [COMPUTE\\_ALL\\_EQUILIBRIA on page 23](#).
- Copy the final values of your optimizing variables and set them as start values of the variables in the setup macro file (with [SET\\_FIX\\_VARIABLE on page 112](#)).



It is important that you round off the values of the optimizing variables correctly. See [Rounding off Optimizing Variable Values on the previous page](#). When you have done this, you can run the setup macro file to recreate the final result of the optimization.

---

## Alternate Mode

In this section:

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<i>About Alternate Mode</i> .....	<a href="#">43</a>
<i>Optimizing in Alternate Mode</i> .....	<a href="#">43</a>
<i>Preparing the POP-file for Alternate Mode</i> .....	<a href="#">44</a>
<i>Examples of SET_ALTERNATE_CONDITION</i> .....	<a href="#">44</a>

## About Alternate Mode

To turn Alternate Mode ON or OFF, use the PARROT command [SET\\_ALTERNATE\\_MODE](#) on page 111.

When you have one or more multi-phase equilibria (that is, with the fixed phase-status) in your POP-file and the optimizing values lack appropriate starting values (such as the default value of 0 for example), then Thermo-Calc may not be able to compute the equilibria for the experiments. In these cases, a common tangent cannot be found, that is, a state where the chemical potentials for all components are the same in all phases cannot be found. A common tangent may not exist or it be found at the wrong composition or temperature given the initial set of model parameters.

If you are not able to estimate reasonable starting values for the optimizing variables, then this problem can be overcome by initially running your optimization in alternate mode. The alternate mode in PARROT module should help you find reasonable starting values for the optimizing variables. Note that you are only supposed to use alternate mode in the beginning of the optimization. Once you have achieved a reasonable fit between calculated results and experimental data, turn off alternate mode and calculate all equilibria again in the normal mode.

In alternate mode, PARROT modifies multi-phase equilibria so that the chemical potentials for each stable phases is calculated separately. For example, consider the following experimental equilibrium:

```
CREATE_NEW_EQUILIBRIUM 1 1
CHANGE_STATUS PHASE LIQ FCC=FIX 1
SET_CONDITION T=1000 P=1E5
EXPERIMENT X(LIQ,B)=.2:.01 X(FCC,B)=.1
```

When PARROT optimizes in alternate mode, the computation of this equilibrium is done by way of the following two calculations:

```
CHANGE_STATUS PHASE LIQ=FIX 1
SET_CONDITION T=1000 P=1E5 X(LIQ,B)=.2
CHANGE_STATUS PHASE FCC=FIX 1
SET_CONDITION T=1000 P=1E5 X(FCC,B)=.1
```

The difference between the chemical potentials in every pair of phases is calculated and PARROT tries to adjust the parameters of the phases so that these differences are minimized. In other words, PARROT tries to make the chemical potentials equal in all phases. For PARROT to be able to do this, some additional information about the experimental multi-phase equilibria is required, at least for all invariant equilibria.

## Optimizing in Alternate Mode

When you are optimizing in the alternate mode, you usually do not need to enter the ED\_EXP module and manually change the weights of experiments that the computed results have not been fitted well with. Instead, after using [OPTIMIZE\\_VARIABLES](#) on page 109 initially with no iterations, and listing the result with [LIST\\_RESULT](#) on page 104, simply run OPTIMIZE\_VARIABLES again specifying, say, thirty

iterations. Continue to optimize until your optimization seems to be going in the right direction, then set the optimizing variables' starting values to their current values use [RESCALE\\_VARIABLES](#) on page 110 before you turn alternate mode off by answering N at the [SET\\_ALTERNATE\\_MODE](#) on page 111 prompt.

## Preparing the POP-file for Alternate Mode

Information in your POP-file that concerns equilibria with ENTERED or DORMANT phases is ignored when you optimize in alternate mode.

To use the alternate mode, ensure that there is enough information about each phase in a given equilibrium. In addition to the temperature and pressure of the system, you should specify the composition of all phases in a given equilibrium. This is done with, [SET\\_CONDITION](#) on page 165, [EXPERIMENT](#) on page 24 or [SET\\_ALTERNATE\\_CONDITION](#) on page 30.

If both compositions of a binary tie-line have been measured, then you could specify this in the POP-file in the following way:

```
CREATE_NEW_EQUILIBRIUM 1 1
CHANGE_STATUS PHASE FCC BCC=FIX 1
SET_CONDITION P=1E5 T=1000
EXPERIMENT X(BCC,B)=.2:.01 X(FCC,B)=.3:.01
```

This equilibrium could be calculated with alternate mode without any modification. The compositions specified with the experiment command is used as condition when the thermodynamic properties of each phase are calculated.

## Examples of SET\_ALTERNATE\_CONDITION

The following topics demonstrate how [SET\\_ALTERNATE\\_CONDITION](#) on page 30 is used to prepare different kinds of equilibria for optimization in alternate mode.



## Specifying the Composition of One Side of a Binary Tie-Line

If only one side of the tie-line has been measured, then you must provide an estimate of the composition of the other phase. You can make such an estimate with SET\_ALTERNATE\_CONDITION. This command has no effect unless alternate mode is turned on. The equilibrium described could thus be specified in the following way:

```
CREATE_NEW_EQUILIBRIUM 1 1
CHANGE_STATUS PHASE FCC BCC=FIX 1
SET_CONDITION P=1E5 T=1000
EXPERIMENT X(BCC,B)=.2:.01
SET_ALTERNATE_CONDITION X(FCC,B)=.3
```

When the alternate mode is turned on, the composition given by the SET\_ALTERNATE\_CONDITION command is used for the FCC phase. The properties of the BCC phase is calculated using the composition specified by experiment as a condition.

## Specifying the Compositions of a Three-Phase Equilibrium

If you have a three-phase equilibrium in your POP-file, then one of its compositions can be specified as experimentally determined, while two can be provided as alternate conditions:

```
CREATE_NEW_EQUILIBRIUM 1 1
CHANGE_STATUS PHASE FCC BCC LIQ=FIX 1
SET_CONDITION P=1E5
EXPERIMENT T=912:5 X(LIQ,B)=0.2:.02
SET_ALTERNATE_CONDITION X(FCC,B)=0.1 X(BCC,B)=.4
```

## Specifying the Composition of a Stoichiometric Phase

When you specify the composition of stoichiometric phase with SET\_ALTERNATE\_CONDITION, the value must be given with at least seven decimal digits, as in the following example:

```
CREATE_NEW_EQUILIBRIUM 1 1
CHANGE_STATUS PHASE LIQ A2B=FIX 1
SET_CONDITION P=1E5 X(LIQ,B)=0.2
EXPERIMENT T=992:5
SET_ALTERNATE_CONDITION X(A2B,B)=.6666667
```

## Entering Other Experiments in the POP with Alternate Mode

The following table shows some additional examples of how to enter different kinds of experiments in the POP-file when you are using the alternate mode.

Example	ED_EXP commands
Two-phase equilibrium: The melting temperature of an Au-Cu alloy	CHANGE_STATUS PHASE LIQUID FCC=FIX 1 SET_CONDITION X (FCC,CU)=0.14 P=1E5 EXPERIMENT T=970:2 SET_ALTERNATE_CONDITION X(LIQUID,CU)=0.16
Invariant equilibrium experiment: A three- phase equilibrium in a binary system	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE FCC BCC LIQUID=FIX 1 SET_CONDITION P=1E5  EXPERIMENT T=912:5 SET_ALTERNATE_CONDITION X(FCC,B)=0.1SET_ ALTERNATE_CONDITION X(BCC,B)=0.4SET_ALTERNATE_CONDITION X (LIQ,B)=0.2
Ternary system, with two compositions measured (both with uncertainty 0.02)	CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE FCC BCC=FIX 1 SET_CONDITION T=1273 P=1E5 SET_CONDITION X(FCC,B)=0.1:0.02 EXPERIMENT X(FCC,C)=0.12:.02 SET_ALTERNATE_CONDITION X (BCC,B)=0.17 SET_ALTERNATE_CONDITION X(BCC,C)=0.07

---

## Troubleshooting

During an optimization, you are likely to run into many different problems and challenges. This topic gives some general guidelines that can help avoid common mistakes and problems.

In this section:

---

<i>Useful Guidelines</i> .....	48
<i>Excluding and Including the Correct Equilibria</i> .....	49
<i>Conflicting Data</i> .....	49

---

## Useful Guidelines

The following rules of thumb are generally good to adhere to when you are planning and executing an optimization:

- Do not use data from thermochemical tables of unknown origin.
- Use experimentally determined properties; avoid converted quantities.
- Carefully estimate the accuracy of the experiments.
- Correct systematic errors (by adjusting a temperature scale for example).
- Use negative information such as, for example, the information that a phase should not be stable in a composition or temperature region.
- With a hundred activity measurements in a system but only ten composition points from the phase diagram, it is often appropriate to decrease the weights on the activity experiments.
- If you initially exclude any intermediate phases to only optimize the liquid and the terminal or end-member phases for the pure components, then it is often useful to compute a metastable phase diagram with just these phases. In the metastable phase diagram, the metastable solubility lines should not have any strange kinks or turns. Such a diagram is often also useful to compute at later stages in the optimization.
- When you have fitted the liquid phase and some solution phases reasonably well, then you can fix the optimizing variables that characterise these phases. You can then go on and optimize the variables for the intermediate phases.
- Phases with miscibility gaps are always difficult to optimize. Try to keep control of the miscibility gaps by using real or estimated experimental information. (Note that it is not possible to calculate the top of a miscibility gap as a single equilibrium.)
- Phases with order/disorder transformation are often difficult to optimize. It may be difficult to find the right start values on the optimizing variables. The `TABULATION` module (see [TABULATION\\_REACTION Commands on page 245](#)) can be useful sometimes. Properties for specified site fractions can be calculated in the `TABULATION` module. This is not possible in the `POLY` module since this module only calculates for equilibrium site fractions. The ordered state may also disappear during the optimization of these phases. If this happens, you may be able to add an experiment that controls the state of order.
- Only use the alternate mode to find an initial set of model parameters that can then be make it possible to calculate the experimental equilibria in the normal mode.
- When you have achieved a satisfactory fit between calculated results and experimental data with an appropriate number of optimization variables, perform a couple of final optimization runs to make sure that your results are stable.

- Make sure that the values of the optimizing variables keep within a reasonable range. If a variable starts to change several orders of magnitudes, then you must consider whether you have the right weights on the experiments and whether you are using too many optimizing variables.

## Excluding and Including the Correct Equilibria

Use as few experiments as possible initially to get a reasonable overall fit. It is generally best to first focus on the invariant equilibria, as well as metastable states that can be estimated by excluding some phases. Crucially, any experiments for which the computed results are clearly faulty should be excluded from the final critical set, while all important invariant equilibria are calculated and included in this critical set.

If you cannot compute some invariant equilibria with intermediate phases, then it may be best to first exclude those phases from the optimization and only optimize the liquid and the most important solution phases. After you have obtained reasonable results for these phases, you can enter the intermediate phases back in again. With the variables for the optimized liquid and solid phases set fixed, you can finally optimize the intermediate phases.

## Conflicting Data

It is important that you do not include conflicting sets of data at the same time during an optimization. After all, if they are genuinely conflicting, then at least one of the sets must be incorrect. If you have conflicting sets of data, then only use one of these sets at a time together with the rest of the data. Often, the optimization makes it clear which dataset coheres best with the other information that is available about the system.

Sometimes, conflicting data cannot be detected directly. For example, you may have activity data which is inconsistent with solubility data from the phase diagram. This would be indicated by large errors in the fit when both the activity data and the solubility data are included. To find these inconsistencies, let alone correct the errors, you may thus have to optimize with some datasets excluded.

---

## Experiments and Experimental Data

These topics contain examples of different kinds of equilibria in different kinds of systems. They are intended to help you figure out how to use various kinds of experimental data when creating POP-files. The topics that follow contain examples how to enter various kinds of experimental data into a POP-file.

In this section:

---

<i>Phase Diagram Data</i> .....	51
<i>Data for Individual Compounds</i> .....	52
<i>Single Phase Mixing Enthalpies or Partial Enthalpies</i> .....	53
<i>Enthalpies of Formation and Enthalpies of Reactions</i> .....	54
<i>Chemical Potentials via EMF Measurements</i> .....	55
<i>Driving Force for Metastable Phases</i> .....	55
<i>Pressure-Temperature-Volume EOS Data</i> .....	56
<i>Crystal Structure, Lattice Parameters and Site-Occupancy</i> .....	56
<i>Magnetism and Other Atomistic Properties</i> .....	57
<i>Data About Systems of Different Orders</i> .....	58

## Phase Diagram Data

P-T-X phase diagram data for binary and ternary systems, or systems of even higher order can be used in the POP-file. This includes data of the following types:

- Data about the temperature- and composition-dependence of various properties (obtained from differential thermal analysis (DTA) measurements for example), including enthalpy, lattice parameter, dilatometric length, electronic conductivity and magnetic susceptibility;
- Data about reaction types (invariant/monovariant) and phase relations obtained from qualitative or quantitative metallographic studies;
- Data about phase amounts or compositions obtained from microprobe measurements (using X-ray spectroscopy or transmission electron microscopy (TEM));
- Data about the positions or directions of two-phase tie-lines and three-phase equilibria for ternary systems.

### Example

The following table shows a POP-file excerpt that demonstrates how some kinds of phase diagram data can be entered:

Example	ED_EXP commands
Solidus (melting temperature) of an Au-Cu alloy	<pre>CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE LIQUID FCC=FIX 1 SET_CONDITION X(FCC,CU)=0.14 P=1E5 EXPERIMENT T=970:2</pre>
Three-phase equilibrium in a binary A-B system	<pre>CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE FCC BCC LIQUID=FIX 1 SET_CONDITION P=1E5 EXPERIMENT T=912:5</pre>
Congruent transformation in a binary A-B system	<pre>CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE BCC LIQUID=FIX 1 SET_CONDITION P=1E5 X(BCC,B)-X(LIQ,B)=0 EXPERIMENT T=1213:10</pre>
Tie-line in a ternary A-B-C system	<p>An uncertainty factor is set not only for the experimental measurement, but also for the X(FCC,B) condition. The factor is 0.02.</p> <pre>CREATE_NEW_EQUILIBRIUM 1 1</pre>

Example	ED_EXP commands
	<pre>CHANGE_STATUS PHASE FCC BCC=FIX 1 SET_CONDITION T=1273 P=1E5 X(FCC,B)=0.1:0.02 EXPERIMENT X(FCC,C)=0.12:.02</pre>

## Data for Individual Compounds

You can use data about individual components in the POP-file. Such data includes activity, heat capacity, heat content, entropy, Gibbs energy of phase transformations, heat of transition and heat of melting.

### Examples

Example	ED_EXP commands
Carbon activity data in the fcc phase	<pre>CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE FCC_A1=FIX 1 CHANGE_STATUS PHASE GRAPHITE=D SET_REFERENCE_STATE C GRAPHITE,,,, SET_CONDITION P=101325 T=1273 X(MN)=0.03 SET_CONDITION X(C)=0.03 EXPERIMENT ACR(C)=0.29:5%</pre>
Ln(activity coefficient for O)	<pre>CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE IONIC_LIQ=FIX 1 CHANGE_STATUS PHASE GAS=D SET_CONDITION X(O)=0.02 T=1523 P=101325 SET_REFERENCE_STATE O GAS,,,, ENTER_SYMBOL FUNCTION LNFO=LOG (ACR(O) / X(O) ); EXPERIMENT LNFO=-1.5:0.01</pre>
Entropy at 298.15 K of Cu <sub>2</sub> O	<pre>CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE CU2O=FIX 1 CHANGE_STATUS PHASE CUO=FIX 0 SET_CONDITION P=101325 T=298.15 EXPERIMENT S=92.36:1</pre>
Gibbs energy of formation of NiAl <sub>2</sub> O <sub>4</sub>	<pre>CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE SPINEL=ENT 1 CHANGE_STATUS PHASE FCC O2GAS=DORM</pre>



Example	ED_EXP commands
	<pre> SET_REFERENCE_STATE NI FCC,,,, SET_REFERENCE_STATE AL FCC,,,, SET_REFERENCE_STATE O O2GAS,,,, SET_CONDITION P=101325 T=1000 N(NI)=1 N(AL)=2 SET_CONDITION N(O)=4 EXPERIMENT GM=-298911:5%</pre>
Heat capacity of MgFe <sub>2</sub> O <sub>4</sub>	<pre> CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE SPINEL=ENT 1 SET_CONDITION P=101325 N(Fe)=2 N(Mg)=1 N(O)=4 SET_CONDITION T=800 ENTER_SYMBOL FUNCTION CP=H.T; EXPERIMENT CP=207:5%</pre>
Heat content (H-H <sub>298</sub> ) for MnFe <sub>2</sub> O <sub>4</sub>	<pre> CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE SPINEL=ENT 1 SET_CONDITION P=101325 T=298.15 N(Mn)=1 N(Fe)=2 SET_CONDITION N(O)=4 ENTER_SYMBOL VAR H298=H; ENTER_SYMBOL FUN HMNFE2O4=H-H298; CREATE_NEW_EQUILIBRIUM 2 1 CHANGE_STATUS PHASE SPINEL=ENT 1 SET_CONDITION P=101325 N(Mn)=1 N(Fe)=2 N(O)=4 SET_CONDITION T=400 EXPERIMENT HMNFE2O4=16610:5%</pre>

## Single Phase Mixing Enthalpies or Partial Enthalpies

You can use calorimetric data for mixing in the POP-file. This data could be the result of, for example, drop calorimetry or scanning calorimetry. This includes data about, for example, enthalpy of mixing of liquids, series of mixing-enthalpy and about partial enthalpy. Information about enthalpies of mixing can also be derived from theoretical principles using special quasi-random structures (SQSs).

### Example

Example	ED_EXP commands
Enthalpy of mixing in the liquid state of an Au-Cu alloy	<pre>CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE LIQUID=FIX 1 SET_CONDITION T=1379 P=1E5 SET_CONDITION X(LIQUID,AU)=0.0563 SET_REFERENCE_STATE AU LIQ * 1E5 SET_REFERENCE_STATE CU LIQ * 1E5 EXPERIMENT HMR=-1520:200</pre>

## Enthalpies of Formation and Enthalpies of Reactions

You can use calorimetric data for phase transformations in the POP-file. This data could be the result of, for example, direct-reaction calorimetry, solution calorimetry or combustion calorimetry. Information about enthalpies of formation can also be derived from theoretical principles.

## Examples

Example	ED_EXP commands
Enthalpy of melting of the eutectic in the Al <sub>2</sub> O <sub>3</sub> -ZrO <sub>2</sub> binary (J/g)	<pre> CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE CORUNDUM ZRO2_TETR=FIX 0 CHANGE_STATUS PHASE IONIC_LIQ=ENT 1 SET_CONDITION P=101325 N=1 LNAC(O)=-80 SET_REFERENCE_STATE ZRO2 TETR,,,,, SET_REFERENCE_STATE AL2O3 CORUND,,,,, EXPERIMENT HWR=1080:90 </pre>
Enthalpy of formation of o-CaZrO <sub>3</sub> from the component oxides	<pre> CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE ZRO2_MONO HALITE CAZRO3_O=ENT 1 SET_CONDITION T=298.15 P=101325 N(CAO)=.5 SET_CONDITION N(ZRO2)=.5 LNAC(O)=-20 SET_REFERENCE_STATE CAO HALITE,,, SET_REFERENCE_STATE ZRO2 ZRO2_MONO,,,, EXPERIMENT HMR(CAZRO3_O)=-15960:5% </pre>

## Chemical Potentials via EMF Measurements

You can use chemical potentials and activities/activity coefficients from electromagnetic field (EMF) measurements in the POP-file.

### Example

Example	ED_EXP commands
Emf data on Cu(s)/Cu <sub>2</sub> O (s)	<pre> CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE FCC CU2O=FIX 1 CHANGE_STATUS PHASE O2GAS=DORM SET_CONDITION P=101325 T=1000 SET_REFERENCE_STATE O O2GAS,, 100000 EXPERIMENT MUR(O)=-95387:1000 </pre>

## Driving Force for Metastable Phases

You can use chemical driving forces for metastable phases in the POP-file.

### Examples

Example	ED_EXP commands
To prevent BCC_A2 to be stable	<pre>CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE FCC_A1 M7C3 M23C6=FIX 1 CHANGE_STATUS PHASE BCC_A2=D SET_CONDITION P=101325 T=1473 EXPERIMENT DGM(BCC)&lt;-0.1:0.1</pre>
To promote CEMENTITE to be stable	<pre>CHANGE_STATUS PHASE BCC M7C3 GRAPHITE=FIX 1 CHANGE_STATUS PHASE CEMENTITE=DORMANT SET_CONDITION P=P0 T=973 EXPERIMENT DGM(CEM)&gt;0.1:0.01</pre>

## Pressure-Temperature-Volume EOS Data

You can use Pressure-Temperature-Volume Equation of State (EOS) data in the POP-file. Such data includes, for example, molar volume, density, thermal expansion and bulk-modulus/compressibility.

### Examples

Example	ED_EXP commands
Volume of liquid Pt	<pre>CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE LIQUID=ENT 1 SET_CONDITION P=101325 N=1 T=1873 EXPERIMENT VM=1.00758E-5:5%</pre>
Thermal expansion	<pre>CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE FCC_A1=ENT 1 SET_CONDITION P=101325 N=1 T=400 ENTER_SYMBOL FUNCTION ALPHA=VM.T/VM/3; EXPERIMENT ALPHA=2.35E-5:5%</pre>

## Crystal Structure, Lattice Parameters and Site-Occupancy

You use information about defects, ordering or site occupancy, as well as information about crystal structures in the form of lattice parameter values. This information may come from measurements made by X-ray, neutron diffraction, Mössbauer spectroscopy or perturbed angular-correlation.

### Examples

Example	ED_EXP commands
Lattice parameter for fcc	<pre> CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE FCC_A1=ENT 1 SET_CONDITION P=101325 N=1 T=298.15 SET_CONDITION X(CR)=0.05 ENTER_SYMBOL FUNCTION LPFCC=((4*VM/6.02214179E23)** (1/3))*1E10; EXPERIMENT LPFCC=4.02:5% </pre>
Lattice parameter for bcc	<pre> CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE BCC_A2=ENT 1 SET_CONDITION P=101325 N=1 T=298.15 SET_CONDITION X(AL)=0.08 ENTER_SYMBOL FUNCTION LPBCC=((2*VM/6.02214179E23)** (1/3))*1E10; EXPERIMENT LPBCC=2.90:5% </pre>
Site-occupancy, degree of inversion for spinel	<pre> CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE SPINEL=ENT 1 SET_CONDITION P=101325 N(MG)=1 N(AL)=2 N(O)=4 SET_CONDITION T=1073 EXPERIMENT Y(SPINEL,AL+3#1)=0.31:5% </pre>

## Magnetism and Other Atomistic Properties

You can use data about atomistic properties such as magnetism and Curie temperatures in the POP-file.

### Example

Example	ED_EXP commands
Curie temperature of $\text{Mn}_x\text{Fe}_{3-x}\text{O}_4$ , $x=1.26$	<pre> CREATE_NEW_EQUILIBRIUM 1 1 CHANGE_STATUS PHASE SPINEL=ENT 1 SET_CONDITION T=520 P=101325 N(O)=4 SET_CONDITION N(Fe)+N(Mn)=3 N(Mn)=1.26 EXPERIMENT TC (SPINEL)=520:5 </pre>

## Data About Systems of Different Orders

You might want to use data about systems of different orders in the same optimization, such as data about a binary equilibrium with components A and B in a ternary system with components A, B and C, together with data about equilibria in the binary system with components A and B. To do this, you must first suspend all components in the ternary system (A, B and C), and then set the two components you want binary information on (A and B) to status ENTERED.

Suspending all components is done by giving the initialization code 0 to the [CREATE\\_NEW\\_EQUILIBRIUM on page 143](#) command. The components about which you want to use binary information must then be entered again using the [CHANGE\\_STATUS on page 59](#) command.

### Example

Example	ED_EXP commands
A binary (A-B) three-phase equilibrium (FCC-BCC-LIQ) in a ternary system (A-B-C)	<pre> CREATE_NEW_EQUILIBRIUM 1 0 CHANGE_STATUS COMPONENT A B = ENTERED CHANGE_STATUS PHASE FCC BCC LIQ=FIX 1 SET_CONDITION P=1E5 EXPERIMENT T=1177:10 </pre>

---

## Thermodynamic Models

The most common models used in assessments are described briefly in these topics. Examples of how to write the phase definitions in the setup-file are also given for each of these models. In addition to the models described here, a large number of thermodynamic models for various phases in different states have been implemented.

In this section:

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<i>Gas</i> .....	60
<i>Compound Energy Formalism</i> .....	60
<i>Substitutional Liquid</i> .....	60
<i>Ionic Two-Sublattice Liquid Model</i> .....	61
<i>Models for Ordered Phases</i> .....	61
<i>4SL Model for FCC, HCP and BCC</i> .....	62
<i>2SL Model for FCC, HCP and BCC</i> .....	63
<i>Magnetic Ordering</i> .....	64
<i>Molar Volumes and High Pressure</i> .....	64
<i>Excess Models</i> .....	65

## Gas

The gaseous mixture phase is usually treated as a substitutional phase without sublattice. In the gaseous mixture phase, there are usually molecules formed, and the number of constituents of the gas phase is often much larger than the number of elements. These complex constituents have to be defined as species. The ideal gas model may handle a gas phase under low pressures (and low temperatures). This implies that the P-V-T relations and thermodynamic properties of pure gaseous species are calculated as for ideal gas, and that there is interaction between gaseous species in the mixture. In a defined system, there may only exist one gaseous mixture phase. Type code **G** is used for the gas phase:

```
ENTER_PHASE GAS G, 1 H,H1O1,H1O2,H2,H2O1,H2O2,O,O2,O3; N N
```

## Compound Energy Formalism

If the atoms are sufficiently different in size, electronegativity or charge, they may prefer different types of sites in the lattice of crystalline solids. In some cases, a solute atom may even occupy interstitial sites between the normal lattice sites. All such phenomena are treated in Thermo-Calc by the sublattice concept. The Compound Energy Formalism (CEF) has proved to be the most general formalism for many different types of solution phases. It is therefore by default applied to various solid solution phases in the Thermo-Calc software package. CEF can also take ionic constraints (charged cation/anion species) into account. For a comprehensive description on the CEF, please see Hillert (2001), Frisk and Selleby (2001), Sundman and Ågren (1981).

Since the CEF is used by default, no special notation is needed in the phase definition, except for ionic phases, where type code **I** is given.

## Examples

Examples of phase definitions in a setup-file using the CEF:

```
ENTER_PHASE SPINEL I, 4 1 2 2 4
    FE+2,FE+3; FE+2,FE+3,VA; FE+2,VA; O-2; N N
ENTER_PHASE SIGMA, 3 10 4 16
    AL,CO,CR,FE,NB; AL,CO,CR,FE,NB; AL,CO,CR,FE,NB; N N
ENTER_PHASE FCC_A1, 2 1 1
    CR,FE,MN; C,N,VA; N N
ENTER_PHASE BCC_A2, 2 1 3
    CR,FE,MN,VA; C,N,VA; N N
```

## Substitutional Liquid

The liquid phase is normally (but not always) modelled as a substitutional phase with no sublattice, which is occupied by two or more constituents. The constituents are normally the elements, but molecules or associates can also be used. Type code **L** is used for the liquid phase.

### Example

```
ENTER_PHASE LIQUID L, 1
```



```

AL,C,CR,FE,MO,NI,SI ; N N
ENTER_PHASE LIQUID L, 1
C,FE,FEO,FEO3/2,NI,NIO ; N N

```

## Ionic Two-Sublattice Liquid Model

Within the framework of the CEF, the ionic two-sublattice liquid (I2SL) model was developed to be used when there is a tendency for ionization in the liquid, which happens in liquid oxides and sulphides for example. The same model can be used both for metallic and oxide melts. At low levels of oxygen, the model becomes equivalent to a substitutional solution model between metallic atoms. Two sublattices are assumed, one containing charged cations and one containing charged anions, neutrals and vacancies. The complication for an ionic liquid is that the numbers of sites on the cation sublattice and anion sublattice vary with the composition to preserve electroneutrality. For a comprehensive description on the I2SL model, see Hillert et al. (1985), Sundman (1991). In these references, the possible excess parameters are also discussed. Type code `Y` is used for the I2SL model.

### Example

Examples of phase definitions in a setup-file:

```

ENTER_PHASE LIQUID Y,
    AL+3,CR+2,FE+2,NI+2; VA; N N
ENTER_PHASE IONIC_LIQ Y,
    CA+2,MG+2; O-2; N N
ENTER_PHASE IONIC_LIQ Y,
    AL+3,CA+2,FE+2,MG+2,SI+4;
    AL02-1,O-2,SIO4-4,VA,FEO3/2,SIO2; N N

```

## Models for Ordered Phases

Some solution phases have chemical order-disorder transformations: for example, the disordered FCC\_A1 phase can transform to the ordered  $L1_2$  or  $L1_0$  structure where the atoms of different kinds occupy different sublattices. In some cases, it may be advantageous and easy to describe such ordered structures as completely different phases; but in some other cases, like the B2-ordered BCC structure in Al-Fe, the disordered and ordered structures must be described as one single phase because the transformation is of second order along a line in temperature and composition.

The ordering can easily be described by the CEF. For instance, an ordered FCC phase with only  $L1_2$  or  $L1_0$  ordering can be efficiently handled by the so-called Two Substitutional-Sublattice Ordering Model (2SL model), while an ordered FCC with both  $L1_2$  and  $L1_0$  ordering must be described with four sublattices using the so-called Four Substitutional-Sublattice Ordering Model (4SL model). Please note that in both these models, all the substitutional constituents must enter into these sublattices. In addition, you may also have one sublattice for interstitials.

Thermo-Calc supports a feature of splitting the parameters of a chemically ordered phase onto two different phase descriptions. This is very convenient. In this way, you can have one phase for all parameters describing the disordered state (the configuration independent state) and in the other phase only those parameters needed to describe the remaining part (the configuration dependent part), that is, the Gibbs energy contribution due to the ordering transformation. This has been implemented in such a way that the contribution from the configuration dependent part is zero when the solution phase is disordered. The optimization of the disordered phase is independent of the order-disorder transformation; the ordering energy is an add-on to the disordered part. This is particularly useful in higher order systems, as an ordered phase can dissolve several elements that have no particular contribution to the actual ordering. The phases Gibbs energy add together by giving this command in the setup-file: [AMEND\\_PHASE\\_DESCRIPTION on page 52](#) <ordered phase> disordered\_part <disordered phase>

Since PARROT does not automatically create new composition sets, it is necessary to create composition sets for both the ordered and disordered phases in the setup-file: Amend\_phase\_description <phase> composition\_sets <new highest set number>,,, ,

### Example

Example of phase definitions for the corresponding disordered and ordered parts in a setup-file:

```
ENTER_PHASE FCC_A1, 2 1 1
      AL, CR, FE, NI; VA; N N
ENTER_PHASE FCC_L12, 3 .75 .25 1
      AL, CR, FE, NI ; AL, CR, FE, NI; VA; N N
AMEND_PHASE_DESCRIPTION FCC_L12 DIS_PART FCC_A1
```

## 4SL Model for FCC, HCP and BCC

Ordered FCC, HCP and BCC solution phases handled by the 4SL model requires four sublattices for substitutional ordering and can additionally have an interstitial sublattice. A 4SL model is especially useful for modelling different kinds of ordered phases that are based on the same disordered phase, such as  $L1_0$  and  $L1_2$  based on FCC\_A1, and B2,  $DO_{19}$ ,  $L2_1$  and B32 based on BCC\_A2 etc.

For ordered FCC or HCP phases, these four substitutional sublattices represent four corners of the regular tetrahedron on these lattices, all of which are the nearest neighbours. These corners are equivalent lattice points, thus all G parameters for each end-member with the same elements, but distributed on different sites, must be identical. It should be emphasized that the end-member energy here represents the ordering energy rather than the formation energy of the compound.

The constraints on the parameters in the 4SL model can be derived based on the symmetry of the lattice:

$$G_{A:B:B:B} = G_{B:A:B:B} = G_{B:B:A:B} = G_{B:B:B:A}$$

$$G_{A:A:B:B} = G_{A:B:A:B} = G_{A:B:B:A} = G_{B:A:A:B} = G_{B:A:B:A} = G_{B:B:A:A}$$

$$G_{B:A:A:A} = G_{A:B:A:A} = G_{A:A:B:A} = G_{A:A:A:B}$$

$$L_{A,B:***} = L_{*:A,B:***} = L_{*:**A,B:***} = L_{*:***A,B}$$

The asterisk \* means that the interaction parameter is independent of the occupation of that sublattice. For the disordered phase to be completely disordered, i.e. that all site fractions are equal on all four sublattices, all constraints must be correct.

For ordered BCC phases, the situation is a bit more complicated, as the four sublattice ordering phase represents an irregular tetrahedron with two pairs of sites that are next nearest neighbours. Thus, for an A-B binary solution phase, with A located on two sublattice sites and B on the other two, the end-member described by  $G_{A:A:B:B}$  has four nearest neighbour bonds between A and B atoms, whereas the end-member described by  $G_{A:B:A:B}$  has two nearest neighbour bonds between A and B atoms and two next nearest neighbour bonds. Many parameters thus have a relation:

$$G_{A:B:B:B} = G_{B:A:B:B} = G_{B:B:A:B} = G_{B:B:B:A}$$

$$G_{B:A:A:A} = G_{A:B:A:A} = G_{A:A:B:A} = G_{A:A:A:B}$$

$$G_{A:A:B:B} = G_{B:B:A:A}$$

$$G_{A:B:A:B} = G_{A:B:B:A} = G_{B:A:A:B} = G_{B:A:B:A}$$

$$L_{A,B:*,*} = L_{*,A,B:*,*} = L_{*,*,A,B} = L_{*,*,*,A,B}$$

The  $G_{A:B:B:B}$  term represents  $DO_3$ ,  $G_{A:A:B:B}$  B2 and the  $G_{A:B:A:B}$  B32 ordering. There are also two kinds of reciprocal interaction parameters:

$$L_{A,B:A,B:*,*}, 0 \dots 9$$

$$L_{A,B:*,*,A,B}, 0 \dots 9$$

Kusoffsky et al. (2001) have shown the influence of different parameters available in the 4SL model applied to fcc ordering. The possibility to use the 4SL model to BCC ordering has been studied by Sundman et al. (2009) in the Al-Fe system.

## 2SL Model for FCC, HCP and BCC

The reason for using a 2SL model instead of a 4SL model is that the calculations are faster, but on the other hand it can only model one kind of ordered phase(s). For instance, it is not possible to model FCC with both  $L1_0$  and  $L2_1$ , or BCC with  $DO_3$  and B2, etc.

In order to get the fully disordered phase to form, constraints are needed as for the 4SL model. For the symmetric phases, e.g. B2 and  $L1_0$ , the relation between parameters are:

$$G_{A:B} = G_{B:A}$$

$$L_{A,B:*,*} = L_{*,A,B}$$

For a 2SL asymmetric model including, but not limited to,  $L1_2$ , more constraints are needed. This model has many complicated relations between the parameters. The relation between the parameters for the 2SL  $L1_2$  model can be derived from a 4SL model. The conversion from 4SL model parameters to 2SL parameters for  $L1_2$  can be found in Dupin et al. (2001) and for  $L1_0$  in Yuan et al. (2012). Higher-order systems with an  $L1_2$  phase modelled with two sublattices require a lot of ternary and some quaternary

interaction parameters in order to make the disordered state stable. These parameters have been derived by e.g. Dupin (1995), also found in Kusoffsky et al. (2001).

Many publications exist on how to model order/disorder transformations using a two-sublattice model, see e.g. Dupin, Ansara (1999), De Keyser et al. (2009).

## Magnetic Ordering

The magnetic contribution to the Gibbs energy is given by a model proposed by Inden (1975) and adapted by Hillert and Jarl (1978), and is described by:

$$G = RT \ln(b+1) f(t)$$

where  $t = T/T_C$ .

The values of the Curie temperature,  $T_C$ , and Bohr magneton number,  $b$ , at a certain composition are then used in an optimization procedure to calculate the contribution to Gibbs energy due to magnetic ordering. Curie temperature and Bohr magneton number are given in the command [ENTER\\_PARAMETER](#) on page 99 for phases that undergo a magnetic transition:

```
AMEND_PHASE_DESCRIPTION BCC_A2 MAGNETIC -1.0 0.4
ENTER_PARAMETER TC(BCC_A2,FE:VA;0) 298.15 +V1; 6000 N
ENTER_PARAMETER BMAGN(BCC_A2,FE:VA;0) 298.15 +V2; 6000 N
```

The arguments -1 and 0.4 specify the values of parameters in the magnetic model: -1 is the antiferromagnetic factor and 0.4 is the structure factor. Usually the antiferromagnetic factor = -1 for bcc and = -3 for fcc (and other non-bcc phases). The structure factor corresponds to the short range order fraction of the enthalpy. This factor is 0.4 for bcc and 0.28 for non-bcc phases.

## Molar Volumes and High Pressure

Including volumes in a thermodynamic database enable calculations of volume changes, volume fraction, lattice mismatch in cubic structures and phase diagrams at increased pressure. Pressure independent volumes can be used up to about 1 GPa. At pressures above 1 GPa the pressure dependence of the volumes must be included by using a proper equation of state (EOS). An EOS has been developed by Lu et al. (2005), based on the EOS from Jacobs and Oonk (2000). Four parameters are used in the implementation of the model in Thermo-Calc:

- $V_0$ : Volume at 1 bar and at reference temperature  $T_0$
- $V_A$ : Integrated thermal expansivity
- $V_K$ : Isothermal compressibility at 1 bar
- $V_C$ : Parameter to fit high pressure data

All parameters can be composition dependent in the same way as all other model parameters in Thermo-Calc. Experimental information about the temperature, pressure and composition dependence of the

volume can be assessed using these model parameters. To evaluate  $V_0$ ,  $V_A$  and  $V_K$  experimental data at 1 bar only are needed.

### Example

Examples on modelling molar volume in a setup-file:

```
ENTER_PARAMETER V0 (BCC_A2, FE:VA;0) 298.15 +V1; 6000 N
ENTER_PARAMETER VA (BCC_A2, FE:VA;0) 298.15 +V2*T+V3*T**2; 6000 N
ENTER_PARAMETER VC (BCC_A2, FE:VA;0) 298.15 +V4+V5*T; 6000 N
ENTER_PARAMETER VK (BCC_A2, FE:VA;0) 298.15 +V6+V7*T; 6000 N
ENTER_PARAMETER V0 (FCC_A1, CR, FE:VA;0) 298.15 +V8; 6000 N
ENTER_PARAMETER VA (FCC_A1, CR, FE:VA;0) 298.15 +V9*(T-298.15); 6000 N
```

## Excess Models

Unless specifically amended, the excess Gibbs energy terms are modelled by the Redlich-Kister-Muggianu Model. Other excess models for the Gibbs energy are also implemented in Thermo-Calc, such as e.g. Kohler and Toop-Kohler extrapolation models.

Thermo-Calc is not restricted to binary interaction parameters. Ternary, quaternary and higher-order interaction parameters can also be used if there is enough information to evaluate these from experimental data. The ternary interaction parameters are identified by the degrees of the so-called ternary L parameter (i.e. 0, 1 and 2) in the command [ENTER\\_PARAMETER on page 99](#). If the parameter is composition-independent, you only need a single interaction parameter with a degree of zero, i.e. only the  $^0L$  term. If there is a ternary composition-dependent interaction parameter, you must enter all three parameters (0,1 and 2). If such a ternary interaction parameter should be zero, then assign it a function which is zero. If the three interaction parameters have the same value, then that is identical to having a composition-independent ternary parameter.

### Example

```
ENTER_PARAMETER L (LIQUID, A, B, C;0) 298.15 +1000; 6000 N
ENTER_PARAMETER L (LIQUID, A, B, C;1) 298.15 +1000; 6000 N
ENTER_PARAMETER L (LIQUID, A, B, C;2) 298.15 +1000; 6000 N
```

is identical to

```
ENTER_PARAMETER L (LIQUID, A, B, C;0) 298.15 +1000; 6000 N
```

This also means that

```
ENTER_PARAMETER L (LIQUID, A, B, C;0) 298.15 +1000; 6000 N
ENTER_PARAMETER L (LIQUID, A, B, C;1) 298.15 +ZERO#; 6000 N
ENTER_PARAMETER L (LIQUID, A, B, C;2) 298.15 +ZERO#; 6000 N
```

is NOT identical to

---

```
ENTER_PARAMETER L(LIQUID,A,B,C;0) 298.15 +1000; 6000 N
```

# Graphical Mode Examples Guide

Version 2016a



## About the Graphical Mode Examples

These examples are for Thermo-Calc in Graphical Mode. There is a separate set of examples for Thermo-Calc Console Mode.

The Graphical Mode examples are stored without calculated results. In Thermo-Calc, open the example file and select the project icon at the top of the **Project** window. Then right-click and select **Perform now**.



Precipitation Module (TC-PRISMA) examples are included in this folder.

You can open the examples from your computer or download from the website.

### Installed Examples

The PDF and example files are also included with your installation in a folder location based on the operating system.



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

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

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



OS	User type	Default directory
Linux	Non root user	home/<user>/Thermo-Calc/<version>
	Root user	usr/local/Thermo-Calc/<version>

### Download from the Website

You can also download the PDF and the example files from the website

1. Go to <http://www.thermocalc.com/>.
2. From the menu, select **Support → Documentation**.
3. Click **Examples** to expand the list.
4. To the right of the example files you want to download, click **Read More**.
5. Click the links to either open a PDF in a browser or to download zipped files containing the examples.

## Examples of Thermo-Calc Activities

### Example 1: Calculating a Single-Point Equilibrium

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

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

The displayed results of the calculation show that the BCC\_A2 (ferrite) and GRAPHITE phases are stable for this set of equilibrium conditions.

File Name	Activity Example
Ex_01_Single-point_equilibrium	Equilibrium Calculator

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

This example shows how the fractions of stable phases vary for an Fe-0.1 mass-% C alloy when the

temperature is varied between 500 and 2000 K. To allow temperature to vary, the corresponding **Axis Definition** check box is selected. In this example, results are displayed graphically using a **Plot Renderer** activity. To get text results a **Table Renderer** activity is used instead.

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

### Example 3: Fe-C Phase Diagrams

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

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

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

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

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

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

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

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

This example shows how to overlay results from two calculations in the same plot. In *Equilibrium Calculator 1* the stable phase diagram is calculated and in *Equilibrium Calculator 2* the metastable. The

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

File Name	Activity Example
Ex_05_Fe-C_stable_and_metastable_phase_diagram	Equilibrium Calculator

### Example 6: Serially Coupled Equilibrium Calculators

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

- In the first example, the final objective is to calculate the equilibrium at 850°C where the mole fractions of the FCC A1 and BCC A2 phases are 0.5 each for an Fe-Cr-C steel with 10% chromium. In Equilibrium Calculator 1 a simple set of equilibrium conditions (temperature, pressure, system size and composition) are used to find a carbon content where only the FCC A1 and BCC A2 phases are stable. The results from this preliminary calculation are displayed in Table Renderer 1.
- In Equilibrium Calculator 2 the carbon content equilibrium condition is replaced by the condition that the numbers of moles of the BCC A2 phase should be 0.5. The final result is displayed in Table Renderer 2. In this case, the final objective is to calculate the solidus temperature of an Fe-Cr-C steel with 10% Cr and 0.01% C.
- In Equilibrium Calculator 3 the state at 2000 K is calculated and the result is displayed in Table Renderer 3.
- In Equilibrium Calculator 4 the temperature equilibrium condition is replaced by the condition *Fix phase / liquid / 0.0*, meaning that liquid should be stable in an amount of zero moles, i.e. the solidus temperature. The final result is displayed in Table Renderer 4.

File Name	Activity Example
Ex_06_Serial_equilibrium_calculators	Equilibrium Calculator

### Example 7: User-Defined Functions

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

can be entered in terms of *Quantities*  $Q1$ ,  $Q2$ ,  $Q3$  etc., or, for using the Thermo-Calc syntax.

File Name	Activity Example
Ex_07_User_defined_functions	Equilibrium Calculator

### Example 8: Scheil and Equilibrium Solidification

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

File Name	Activity Example
Ex_08_Scheil_and_equilibrium_solidification	Scheil Calculator

### Example 9: Carbide Driving Force Heat Maps

This is an example of using *property grid* calculations to plot the driving force for a carbide as a function of two composition variables. With the property grid calculation type, a 2D grid is generated from the two calculation axes. After the calculation is done, an equilibrium is calculated in each grid point. A Plot Renderer connected to a property grid calculator plots the z-axis property for each equilibrium as a function of the two calculation axes. The final plot can be either a heat map or a contour plot.

File Name	Activity Example
Ex_09_Heat_map_of_carbide_driving_force	Plot Renderer

### Example 10: Phase Transition

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

File Name	Activity Example
Ex_10_Phase_Transition	Property Model Calculator

### Example 11: Coarsening and Interfacial Energy

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

File Name	Activity Example
Ex_11_Coarsening_and_Interfacial_energy	Property Model Calculator

### Example 12: Driving Force and Interfacial Energy

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

File Name	Activity Example
Ex_12_Driving_force_and_Interfacial_energy	Property Model Calculator

## Precipitation Calculator Examples



Examples 13 and 16 are available to all users. The other examples require a Precipitation Module (TC-PRISMA) license to calculate and plot results.



All examples use demonstration database packages included with your installation.

### Example 13: Isothermal Precipitation of $Al_3Sc$

This example simulates the kinetics of precipitation of  $Al_3Sc$  from an FCC\_A1 solution phase. The simulation results can be compared with experimental data collected from Marquis and Seidman<sup>1</sup> and Novotny and Ardell<sup>2</sup>.

#### Details and Plot Example

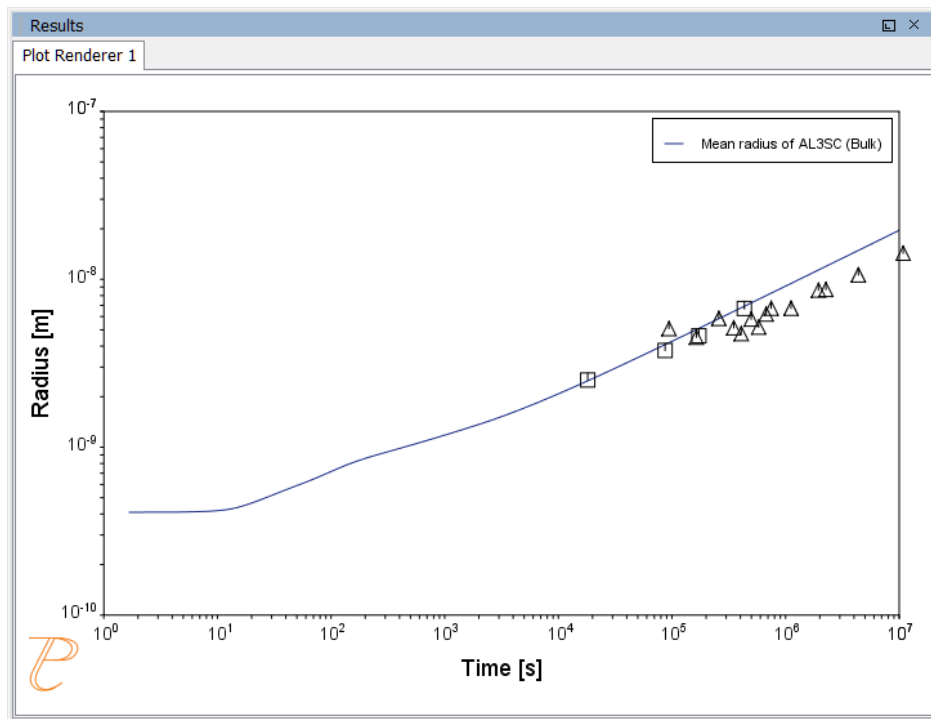
System	
Database package	Demo: Aluminum-based alloys (ALDEMO, MALDEMO)
Elements	Al, Sc
Matrix phase	FCC_A1

<sup>1</sup>E. Marquis, D.. Seidman, Nanoscale structural evolution of  $Al_3Sc$  precipitates in Al(Sc) alloys, Acta Mater. 49 (2001) 1909–1919.

<sup>2</sup>G.M. Novotny, A.J. Ardell, Precipitation of  $Al_3Sc$  in binary Al–Sc alloys, Mater. Sci. Eng. A Struct. Mater. Prop. Microstruct. Process. 318 (2001) 144–154.

Precipitate phases	AL3SC
<b>Conditions</b>	
Composition	Al-0.18Sc Mole percent
Temperature	350° C
Simulation time	1.0E7 seconds
Nucleation sites	Bulk
<b>Precipitate Phase Data Parameters</b>	
Interfacial energy	Calculated
<b>Other</b>	
Calculation type	Isothermal
File name	Ex_13_Precipitation_Al-Sc_AL3SC.tcu

### Plot Results



## Example 14: Stable and Metastable Carbides - Isothermal



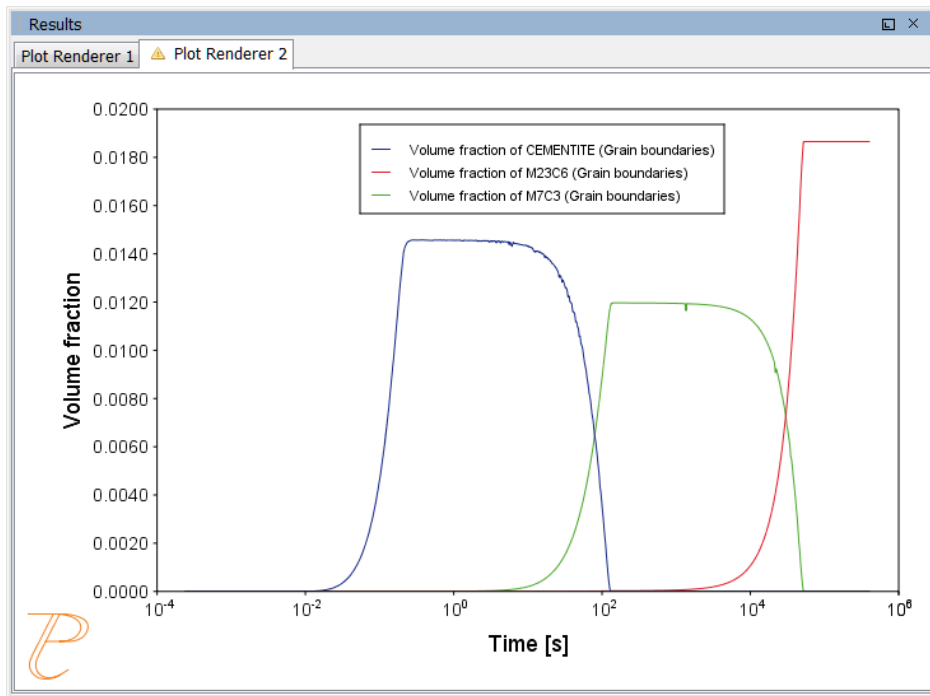
This example simulates the kinetics of precipitation of both stable and metastable carbides from ferrite phase. It demonstrates that metastable carbides (cementite, M7C3) may first emerge and then disappear and the stable phase (M23C6) prevails.

### Details and Plot Example

This example uses the Equilibrium Calculator and a property diagram to determine how the phases change with temperature. We are interested in the carbide precipitation at 1053K where only the carbide M23C6 is stable according to the equilibrium calculation. The Precipitation Calculator is used to do an isothermal calculation of the three phases (cementite, M23C6 and M7C3) where cementite and M7C3 are metastable phases.

System	
Database package	Demo: Steels and Fe-alloys (FEDEMO,MFEDEMO)
Elements	Fe, C, Cr
Matrix phase	BCC_A2
Precipitate phases	Cementite, M23C6 and M7C3
Conditions	
Composition	Fe-0.1C-12Cr Mass percent
Temperature	1053 K
Simulation time	400 000 seconds
Nucleation sites	Grain boundaries
Matrix Phase Data Parameters	
Grain radius	1.0E-4 m
Precipitate Phase Data Parameters	
Interfacial energy	Cementite 0.174 J/m <sup>2</sup> , M23C6 0.26 J/m <sup>2</sup> , M7C3 0.3 J/m <sup>2</sup>
Other	
Calculation type	Isothermal
File name	Ex_14_Precipitation_Fe-C-Cr_Cementite-M7C3-M23C6

## Plot Results



### Example 15: Stable and Metastable Carbides - TTT Diagram

In this example, the kinetics of precipitation of both stable and metastable carbides is calculated from the ferrite phase. It demonstrates that metastable carbides may first emerge and then disappear and the stable phase prevails.

#### Details and Plot Example

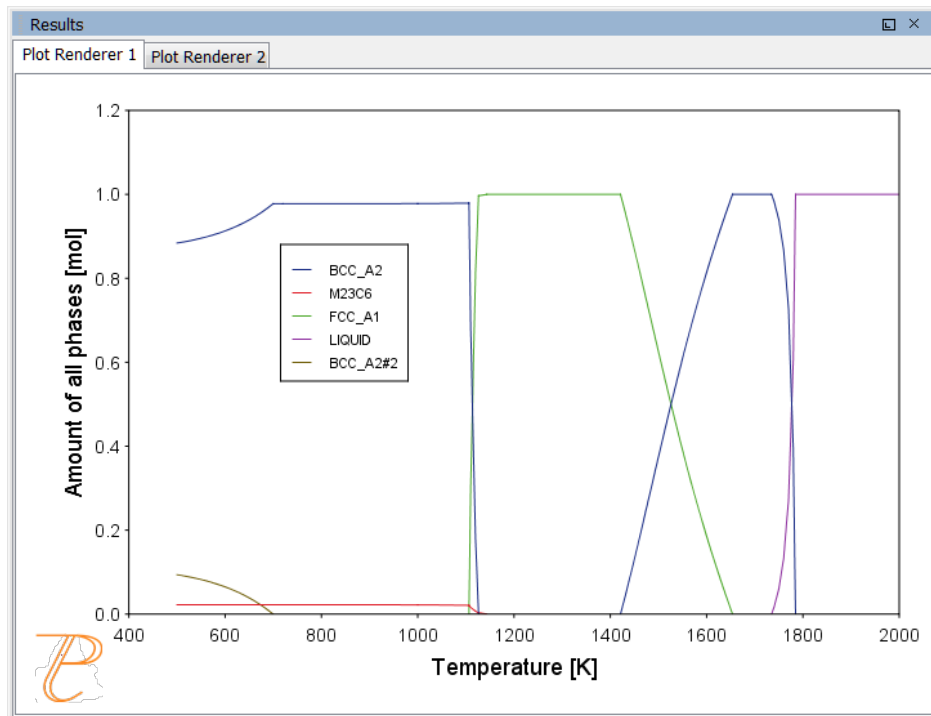
This example uses the Equilibrium Calculator and a property diagram to determine how the phases change with temperature. Using this result, the Precipitation Calculator is used to do a TTT (Time-Temperature-Transformation) diagram calculation of the three phases (cementite, M23C6 and M7C3) at the grain boundaries.

System	
Database package	Demo: Steels and Fe-alloys (FEDEMO,MFEDEMO)
Elements	Fe, C, Cr
Matrix phase	BCC_A2



Precipitate phases	Cementite, M23C6 and M7C3
<b>Conditions</b>	
Composition	Fe-0.1C-12Cr Mass percent
Temperature	500° to 800° C with 25°C steps
Max. simulation time	1.0E8 seconds
Nucleation sites	Grain boundaries
<b>Matrix Phase Data Parameters</b>	
Grain radius	1.0E-4 m
<b>Precipitate Phase Data Parameters</b>	
Interfacial energy	Cementite 0.174 J/m <sup>2</sup> , M23C6 0.26 J/m <sup>2</sup> , M7C3 0.3 J/m <sup>2</sup>
<b>Other</b>	
Calculation type	TTT diagram
Stop criterium	Volume fraction of phase is set to 0.0001
File name	Ex_15_Precipitation_Fe-C-Cr_TTT_Cementite-M7C3-M23C6

## Plot Results



## Example 16: Precipitation of Iron Carbon Cementite

Simulate the kinetics of precipitation of carbides from a BCC Fe solution phase. This example is based on Wert (1949)<sup>1</sup>.

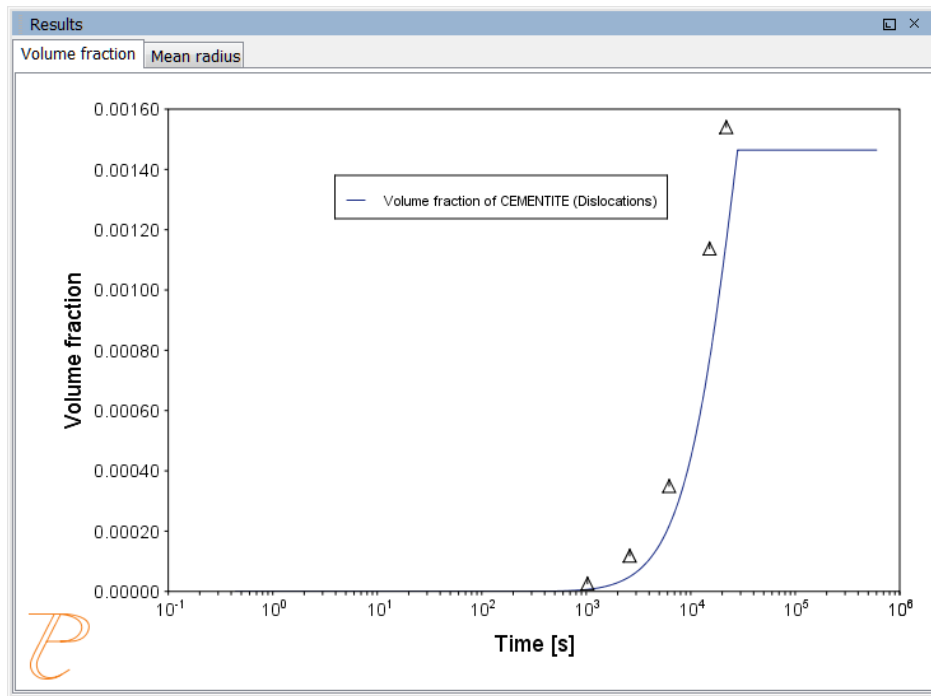
### Details and Plot Example

This example uses two Experimental File Reader activities with the Precipitation Calculator and an isothermal calculation, to plot the volume fraction of the cementite phase.

System	
Database package	Demo: Steels and Fe-alloys (FEDEMO,MFEDEMO)
Elements	Fe, C
Matrix phase	BCC_A2
Precipitate phase	Cementite
Conditions	
Composition	Fe-0.016C mass percent
Temperature	102° C
Simulation time	600 000 seconds
Nucleation sites	Dislocations
Matrix Phase Data Parameters	
Grain aspect ratio	1.0
Precipitate Phase Parameters	
Interfacial energy	0.24 J/m <sup>2</sup>
Dislocation density	1.5e11m <sup>-3</sup>
Other	
Calculation type	Isothermal
Growth rate model	Advanced (on the Options tab)
File name	Ex_16_Precipitation_Fe-C_Cemetite

<sup>1</sup>Wert, C. A. (1949). Precipitation from Solid Solutions of C and N in  $\alpha$ -Iron. Journal of Applied Physics, 20(10), 943.

## Volume Fraction



### Example 17: Precipitation of $\gamma'$ in Ni Superalloys - Isothermal

This example simulates the kinetics of precipitation of  $\gamma'$  phase from  $\gamma$  phase. The simulation results can be compared with experimental data collected from Sudbrack et al.<sup>1</sup>.

#### Details and Plot Examples

This example uses three Experimental File Reader activities with the Precipitation Calculator. It does an isothermal calculation to plot the volume fraction, mean radius and number density of the cementite phase.



DIS\_FCC\_A1 needs to be selected on the System Definer. Search the online help for **About Ordered Phases** in the *Precipitation Module (TC-PRISMA) User Guide* for details.

#### System

Database package

Demo: Nickel-based Super Alloys (NIDEMO and MNIDEMO)

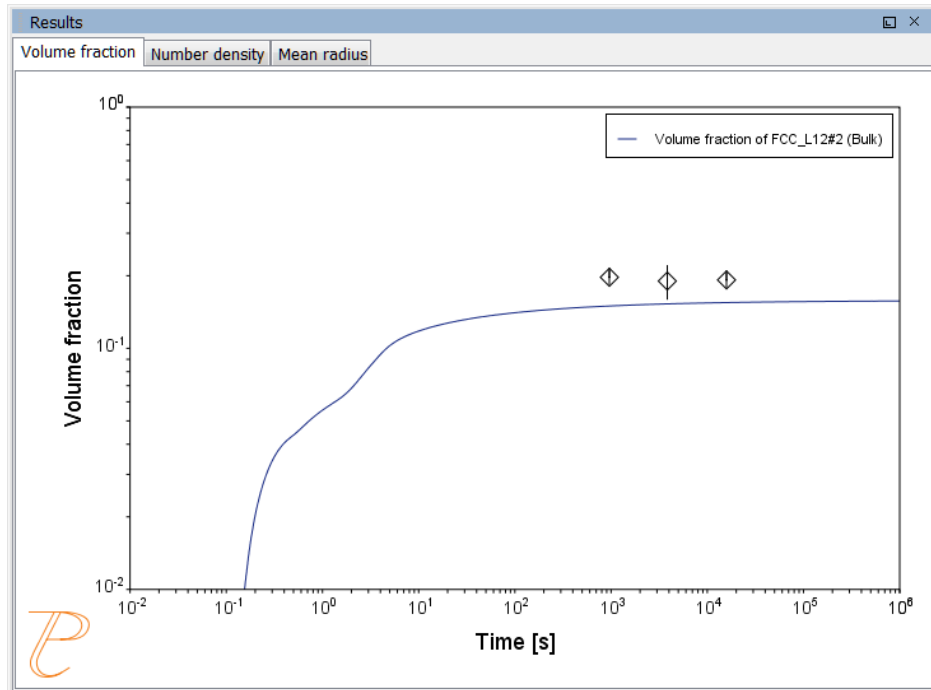
Elements

Ni, Al Cr

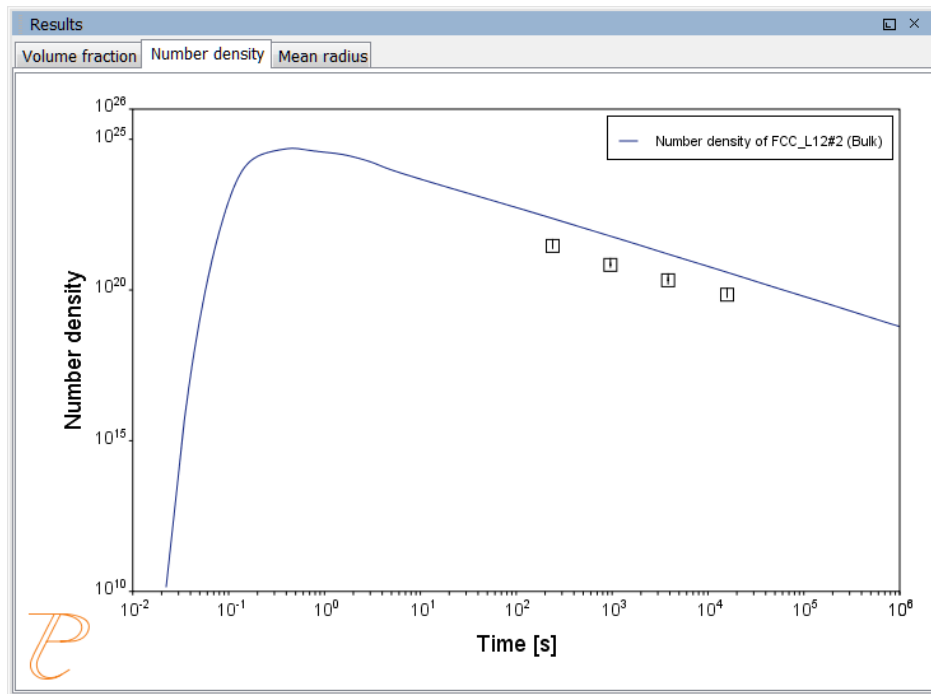
<sup>1</sup>C.K. Sudbrack, T.D. Ziebell, R.D. Noebe, D.N. Seidman, Effects of a tungsten addition on the morphological evolution, spatial correlations and temporal evolution of a model Ni–Al–Cr superalloy, *Acta Mater.* 56 (2008) 448–463.

Matrix phase	DIS-FCC_A1 (see note above about how to select this phase)
Precipitate phase	FCC_L12#2
<b>Conditions</b>	
Composition	Ni-9.8Al-8.3Cr Mole percent
Temperature	800° C
Simulation time	1 000 000 seconds
Nucleation sites	Bulk
<b>Precipitate Phase Data Parameters</b>	
Interfacial energy	0.023 J/m <sup>2</sup>
<b>Other</b>	
Calculation type	Isothermal
File name	Ex_17_Precipitation_Ni-Al-Cr_Isothermal_Gamma-Gamma_prime

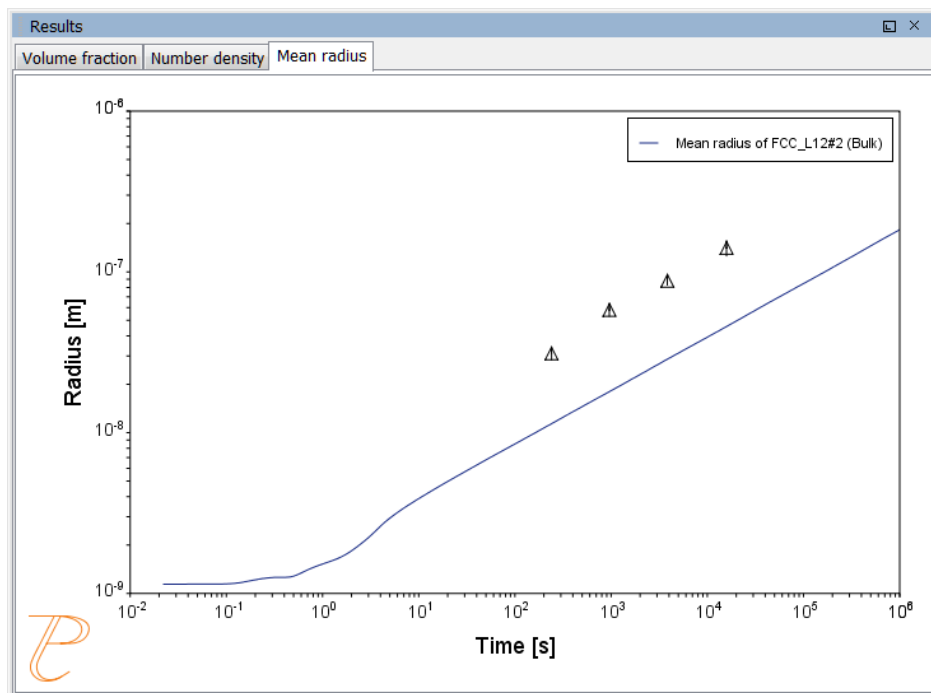
### Volume Fraction



## Number Density



## Mean Radius



## Example 18: Precipitation of $\gamma'$ in Ni Superalloys - Non-isothermal



This example simulates the kinetics of precipitation of  $\gamma'$  phase from  $\gamma$  phase in Ni-8Al-8Cr and Ni-10Al-10Cr at.% alloys during continuous cooling. The simulation results can be compared with experimental results from Rojhirunsakool et al.<sup>1</sup>.

### Details and Plot Examples

In these examples the Separate multimodal PSD check box is selected on the Plot Render to plot the mean radius and size distributions of the two compositions.

Plotting the size distribution from the final simulation time of 1470 seconds, you can see there are several peaks, although these are not completely separated. Use the 'Separate multimodal PSD' check box on the Plot Renderer to separate the peaks. Then adjust the Valley depth ratio setting to 0.05 to separate into two peaks as shown in the [Ni-10Al-10Cr plot example](#). You can experiment with this setting to see how the size distribution evolves with time, for example, try entering several values as plot times '400 600 1470'.



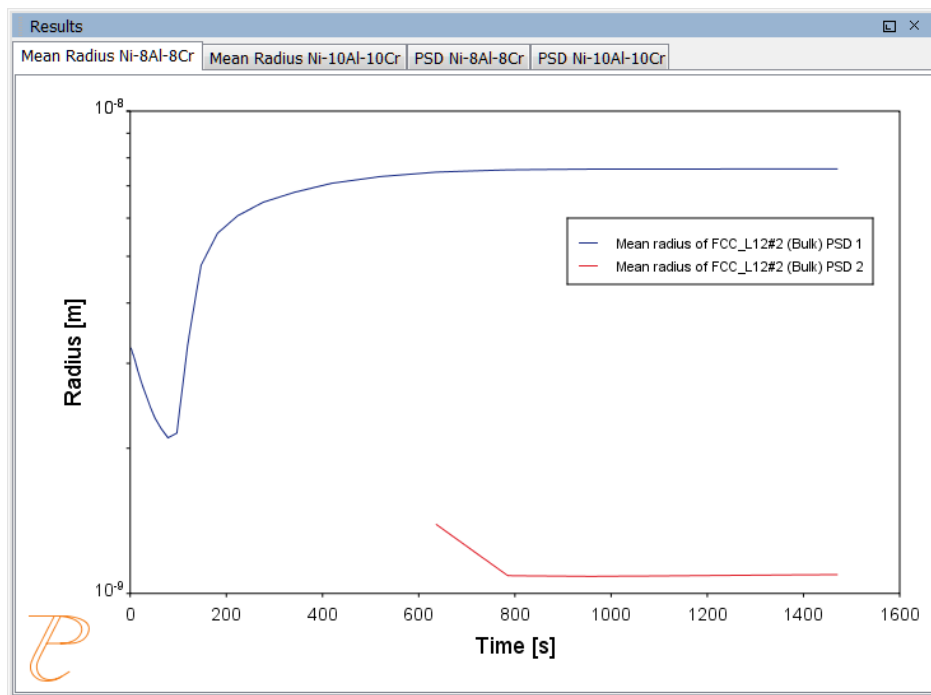
DIS\_FCC\_A1 needs to be selected on the System Definer. Search the online help for **About Ordered Phases** in the *Precipitation Module (TC-PRISMA) User Guide* for details.

System	
Database package	Demo: Nickel-based Super Alloys (NIDEMO and MNIDEMO)
Elements	Ni, Al, Cr
Matrix phase	DIS_FCC_A1 (see note above about how to select this phase)
Precipitate phase	FCC_L12#2
Conditions	
Composition (Ni-8Al-8Cr)	Ni-8Al-8Cr Mole percent
Composition (Ni-10Al-10Cr)	Ni-10Al-10Cr Mole percent
Temperature	0.23 K/s cooling rate
Simulation time	1470 s (Ni-8Al-8Cr), 3300 s (Ni-10Al-10Cr)

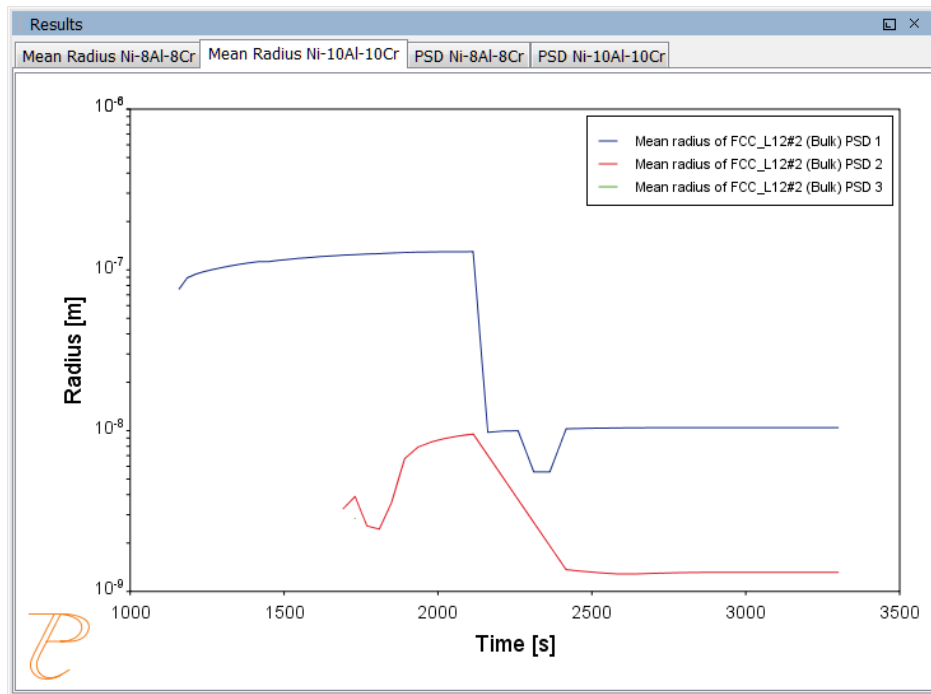
<sup>1</sup>T. Rojhirunsakool, S. Meher, J.Y. Hwang, S. Nag, J. Tiley, R. Banerjee, Influence of composition on monomodal versus multimodal  $\gamma'$  precipitation in Ni–Al–Cr alloys, J. Mater. Sci. 48 (2013) 825–831.

Nucleation sites	Bulk
<b>Matrix Phase Data Parameters</b>	
Mobility enhancement prefactor	5.0
<b>Precipitate Phase Data Parameters</b>	
Interfacial energy	0.023 J/m <sup>2</sup>
<b>Other</b>	
Calculation type	Non-isothermal
Separate multimodal PSD for 8Al-8Cr	On the Plot Renderer, the Valley depth ratio is set to 0.05 for both plots. The number of points is increased to 200 for an average radius plot.
Separate multimodal PSD for 10Al-10Cr	On the Plot Renderer, the Valley depth ratio is set to 0.18 for both plots.
File name	Ex_18_Precipitation_Ni-Al-Cr_Non-isothermal_Gamma-Gamma_prime

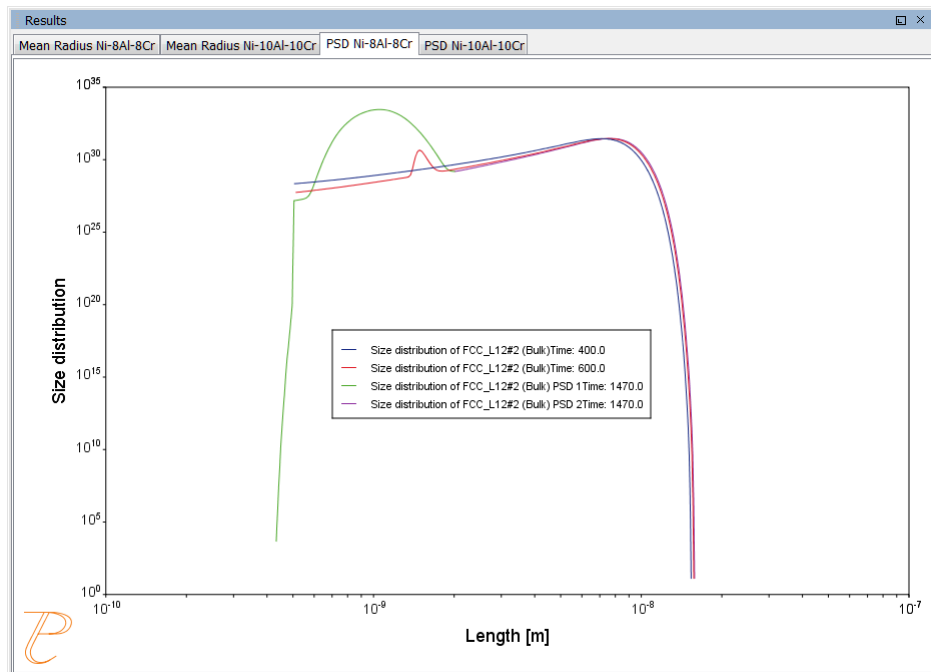
### Mean Radius Ni-8Al-8Cr



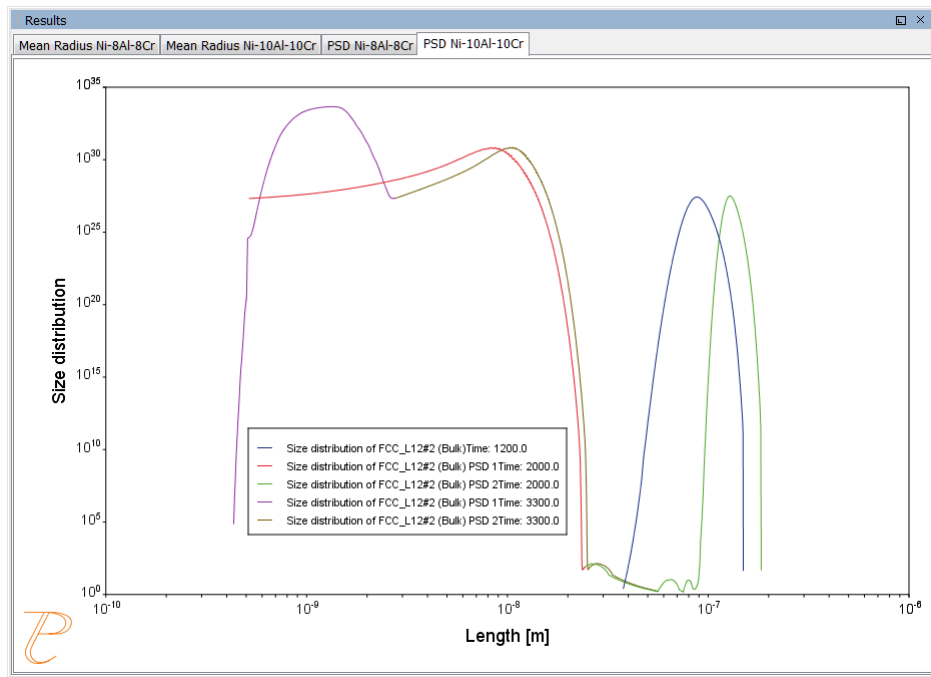
## Mean Radius Ni-10Al-10Cr



## Size Distribution (PSD) Ni-8Al-8Cr

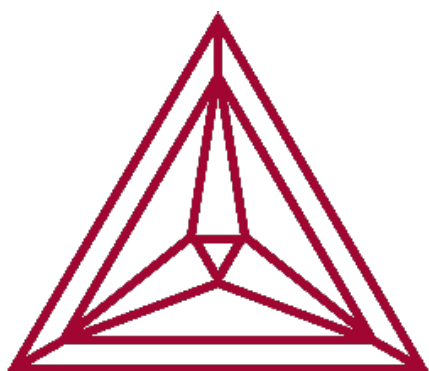




**Size Distribution (PSD) Ni-10Al-10Cr**

# **Console Mode Examples Guide**

**Version 2016a**



## About the Console Mode Examples Guide



This guide is [available as a PDF](#).

For descriptions of each example, see *Console Mode Example Collection* on page 14.

### Installed Examples

The PDF and example files are also included with your installation in a folder location based on the operating system.



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

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

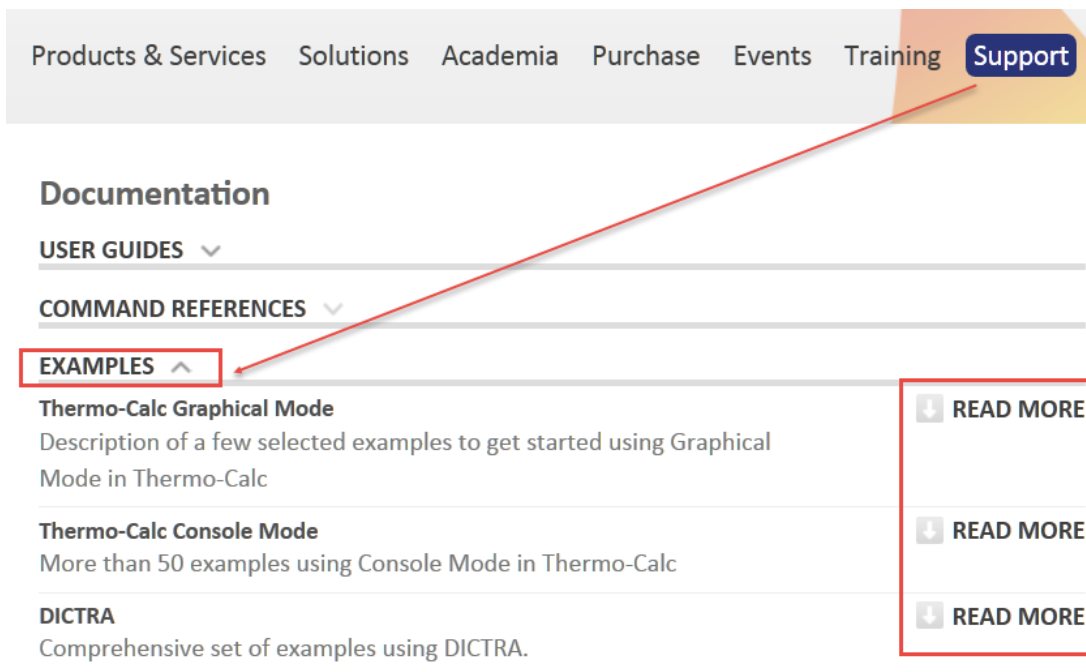
OS	User type	Default directory
Windows	Normal user	Users\<user>\Thermo-Calc\<version> Users\<user>\Documents\Thermo- Calc\<version> My documents
	Administrator	Program Files\Thermo-Calc\<version> Users\Public\Documents\Thermo- Calc\<version> Public documents
Mac	Administrator (user name and password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

### Download from the Website

You can also download the PDF and the example files from the website

1. Go to <http://www.thermocalc.com/>.

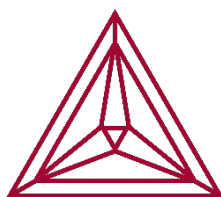
2. From the menu, select **Support** → **Documentation**.
3. Click **Examples** to expand the list.
4. To the right of the example files you want to download, click **Read More**.
5. Click the links to either open a PDF in a browser or to download zipped files containing the examples.





## Console Mode Examples Guide

Thermo-Calc Version 2016a



#### [tcex01](#)

Calculation of the Fe-C binary phase diagram.

#### [tcex02](#)

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

#### [tcex03](#)

Calculation of an isothermal section using TERNARY module

#### [tcex04](#)

Calculation of the miscibility gap in Fe-Cr

#### [tcex05](#)

Calculation of a vertical section in the Al-Cu-Si system Calculation of a vertical section from Al to 10% cu2Si

#### [tcex06](#)

Calculation of an isopleth in low alloyed Fe-Mn-Si-Cr-Ni-C steel. Calculation of a multicomponent phase diagram.

#### [tcex07](#)

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

#### [tcex08](#)

Calculation of a property diagram for a high speed steel i.e. phase fraction plots, activity vs temperature etc.

#### [tcex09](#)

Calculation of dew point

#### [tcex10](#)

Preventing clogging of Cr2O3 in a continuous casting process

#### [tcex11](#)

Oxidation of Cu2S with H2O/O2 gas

#### [tcex12](#)

Tabulation of thermodynamic data for reactions

#### [tcex13](#)

Calculation of phase diagram and G curve using the BINARY module

#### [tcex14](#)

Calculation of the variation of the heat and the heat capacity during solidification of an Al-Cu-Si alloy

#### [tcex15](#)

This is an example of a solidification simulation of a Cr-Ni alloy. No back diffusion in the solid, i.e. Scheil-Gulliver model.

#### [tcex16](#)

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

#### [tcex17](#)

Calculation of the pseudo-binary system CaO-SiO2 using the ionic database

#### [tcex18](#)

Calculation of the A3 temperature of a steel and the influence of each alloying element on this temperature

#### [tcex19A](#)

Mapping of univariant equilibria with the liquid in Al-Cu-Si Part A: step-by-step calculation

#### [tcex19B](#)

Mapping of univariant equilibria with the liquid in Al-Cu-Si Part B: using TERNARY module

#### [tcex20](#)

Example showing how to calculate an adiabatic decompression using the geochemical database

#### [tcex21](#)

Demonstrates the use of a user-defined database, calculate a ternary isotherm in Fe-Cr-Ni.

#### [tcex22](#)

Calculation of a heat balance. In this case C3H8 is burned in oxygen and the adiabatic flame temperature is calculated.

#### [tcex23](#)

Calculation of T-zero and paraequilibria in a low alloyed steel

#### [tcex24](#)

Simulation of the silicon arc furnace using the REACTOR module

#### [tcex25](#)

Simulation of steel refining

#### [tcex26](#)

Plotting of the partial pressure of gas species along the solubility lines in the As-Ga Phase diagram

#### [tcex27](#)

Example of CVD calculation

[tcex28](#)

Example showing calculation of PRE (Pitting Resistance Equivalence) for a duplex stainless steel

[tcex29](#)

Calculation of speciation of a gas

[tcex30A](#)

Example of Scheil calculation for Al-4Mg-2Si-2Cu Part A: step-by-step calculation

[tcex30B](#)

Example of Scheil calculation for Al-4Mg-2Si-2Cu Part B: using SCHEIL module

[tcex31](#)

Calculations of CVM and comparisons with sublattices of a fictitious A B system. Also shows how to overlay diagrams from two calculations

[tcex32](#)

Calculation of oxide layers on steel and show how to append databases

[tcex33](#)

Benchmark calculation for Fe-Cr-C isopleth

[tcex34](#)

Calculation of the phase diagram and G curves in the Al-Zn system

[tcex35](#)

Example of use of the POTENTIAL module

[tcex36a](#)

Assessment. The use of the PARROT module

[tcex37](#)

Calculation of an isothermal section, using command-lines

[tcex38](#)

Calculation of the Morral "rose"

[tcex39](#)

The Calculation of the Reversible Carnot Cycle of Heat Engine

[tcex40](#)

POURBAIX module

[tcex41](#)

Calculation of a solubility product

[tcex42](#)

Paraequilibrium calculation - Formation of Para-pearlite - Isopleth

[tcex43](#)

Paraequilibrium calculation - Formation of Para-pearlite - Isothermal

[tcex44](#)

Exploring the usage of variables and functions. Proof strength for an austenitic stainless steel at elevated temperatures.

[tcex45](#)

3D-Diagram with the gamma volume in the Fe-Cr-C system

[tcex46](#)

3D-Diagram with the liquidus surface of the Fe-Cr-C system

[tcex47](#)

3D-Diagram A quaternary diagram with the gamma volume in the Fe-Cr-Ni-C system at 1373K

[tcex48](#)

Scheil solidification with C back diffusion in solid phases and comparison with simple Scheil and equilibrium calculations.

[tcex49](#)

Quasichemical Model via GES

[tcex50](#)

Quasichemical Model via TDB

[tcex51](#)

Calculation of molar volume, thermal expansivity and density.

[tcex52](#)

Changing the excess models for interaction parameters in a solution phase

[tcex53](#)

Pourbaix Diagram Calculations through the TDB-GES-POLY-POST routine

## tcex01

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

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software (build 9533) running on WinNT 64-bit wordlength  
Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118  
License library version: 8.5.1.0017  
Linked: Mon May 16 09:31:44 2016

```
SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex01\tcex01.TCM" set-echo
```

```
SYS: @@
```

```
SYS: @@
```

```
SYS: @@ Calculation of the Fe-C binary phase diagram.
```

```
SYS: @@
```

```
SYS: set-log ex01,,,
```

```
SYS:
```

```
SYS: @@ The log file is set to get command echo.
```

```
SYS: @@ The menu is shown by typing a question mark "?"
```

```
SYS: ?
```

```
... the command in full is HELP
```

ABOUT	HP_CALCULATOR	SET_LOG_FILE
BACK	INFORMATION	SET_PLOT_ENVIRONMENT
CLOSE_FILE	MACRO_FILE_OPEN	SET_TC_OPTIONS
DISPLAY_LICENSE_INFO	OPEN_FILE	SET_TERMINAL
EXIT	SET_COMMAND_UNITS	STOP_ON_ERROR
GOTO_MODULE	SET_ECHO	
HELP	SET_INTERACTIVE_MODE	

```
SYS: @@ When you give a command the program may ask questions.
```

```
SYS: @@ You may obtain help for each question by typing a ? .
```

```
SYS: @@ If you accept the default answer suggested /within slashes/
```

```
SYS: @@ just press "return"
```

```
SYS: info
```

```
... the command in full is INFORMATION
```

```
WHICH SUBJECT /PURPOSE/: ?
```

```
WHICH SUBJECT
```

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

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

```
WHICH SUBJECT /PURPOSE/:
```

```
PURPOSE
```

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

```
*****
```

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

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

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

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

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

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



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

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

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

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

The following commands are available in the SYS module:

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

Notes for versions since TCCR:

- \* Five SYS commands have been taken away from the SYS-Module monitor (and also eliminated from this chapter in the TCCR User's Guide), because they are normally for system debugging purpose only, or obsolete now, or totally irrelevant. Such commands include: NEWS, LIST\_FREE\_WORKSPACE, PATCH, SET\_ERROR\_MESSAGE\_UNIT and TRACE.
- \* The Section 14.3 (Display of General Information) has been completely removed from this chapter since the TCCR User's Guide. However, for the purpose of obtaining information about various subjects in the SYS module, please use the on-line help feature of the TCCR software, i.e., typing the INFORMATON <SUBJECT> command sequence in the SYS module, that will follow a display on screen of some brief information on a certain subject related to the Thermo-Calc software/database/interface package.
- \* The FOP Module (FUNC\_OPT\_PLOT, the simple function optimizer and plotting facility; for function/parameter mathematic-fitting and plotting) has been completely eliminated from the TCCR software. One should instead use the PARROT module to perform critical thermodynamic assessments.
- \* In the meantime, the SYS command SET\_ECHO (that has been blindly existing in the TCC and DICTRA software for a very long time) is documented in the current edition of this chapter in the TCCR User's Guide; see Section 14.2.6 and 14.2.8.

Revision History of the SYS Module User's Guide:

```
=====
Mar 1985  First release
          (Edited by Bo Sundman)
Oct 1993  Second revised release
          (Edited by Bo Sundman)
Sept 1996 Third revised release
          (Edited by Mikael Schalin and Bo Sundman)
Jun 2000  Fourth revised and extended release
          (Edited by Pingfang Shi)
Nov 2002  Fifth revised release
          (Edited by Pingfang Shi)
Jun 2004  Sixth revised and extended release
          (Edited by Pingfang Shi)
Aug 2006  Seven revised and simplified release
          (Edited by Pingfang Shi)
```

**WHICH SUBJECT:**

**SYS:Hit RETURN to continue**

**SYS:** @@ For a binary phase diagram calculation we use the binary module

**SYS:** go  
... the command in full is GOTO\_MODULE

**MODULE NAME:** ?

NO SUCH MODULE, USE ANY OF THESE:

SYSTEM UTILITIES  
GIBBS\_ENERGY\_SYSTEM  
TABULATION\_REACTION  
POLY\_3  
DICTRA\_MONITOR  
BINARY\_DIAGRAM\_EASY  
DATABASE\_RETRIEVAL  
DIC\_PARROT  
REACTOR\_SIMULATOR\_3  
PARROT  
POTENTIAL\_DIAGRAM  
SCHEIL\_SIMULATION  
OLD\_SCHEIL\_SIM  
POURBAIX\_DIAGRAM  
TERNARY\_DIAGRAM

**MODULE NAME:** BIN

THERMODYNAMIC DATABASE module  
Current database: Steels/Fe-Alloys v8.0

```
VA_DEFINED  
L12_FCC          B2_BCC          B2_VACANCY  
HIGH_SIGMA      DICTRA_FCC_A1    REJECTED
```

Simple binary phase diagram calculation module

**Database:** /TCBIN/: TCBIN

Current database: TC Binary Solutions v1.1

```
VA /- DEFINED
BCC_B2 FCC_L12 FCC_L102
D021_HCP REJECTED
First element: fe
Second element: c
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/: Phase-Diagram
... the command in full is REJECT
VA /- DEFINED
BCC_B2 FCC_L12 FCC_L102
D021_HCP REJECTED
REINITIATING GES5 .....
... the command in full is DEFINE_ELEMENTS
C FE DEFINED
LIQUID:L IONIC_LIQUID:Y FCC_A1
BCC_A2 A2_BCC HCP_A3
HCP_ZN DIAMOND_A4 GRAPHITE_A9
CBCC_A12 CUB_A13 B2_FEPD
C14_LAVES C15_LAVES D011_CEMENTITE
D82_FEZN_GAMMA L12_FEPD3 AL5FE4
FE3AS2 FEZN4 FEZN_DELTA
FEZN_ZETA REJECTED
LIQUID:L RESTORED
FCC_A1 RESTORED
BCC_A2 RESTORED
D011_CEMENTITE RESTORED
GRAPHITE_A9 RESTORED
DIAMOND_A4 RESTORED
... the command in full is GET_DATA
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....
```

List of references for assessed data

```
'A T Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4 p 317-425; '
'P Gustafson, Scan J Metall 14(1985) p 259-267; C-Fe'
```

-OK-

```
... the command in full is SET_AXIS_VARIABLE
The condition X(Fe)=.1234 created
... the command in full is SET_AXIS_VARIABLE
The condition T=1319.08 created
... the command in full is SET_REFERENCE_STATE
... the command in full is SET_REFERENCE_STATE
... the command in full is SAVE_WORKSPACES
... the command in full is SET_CONDITION
... the command in full is SET_ALL_START_VALUES
Forcing automatic start values
Automatic start values will be set
... the command in full is COMPUTE_EQUILIBRIUM
... the command in full is COMPUTE_EQUILIBRIUM
Start points provided by database
... the command in full is SAVE_WORKSPACES
Version S mapping is selected
```

Organizing start points

```
Generating start point 1
Generating start point 2
```

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

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

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

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

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

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

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

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

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

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

Phase region boundary 11 at: 9.841E-01 1.011E+03  
 BCC\_A2  
 \*\* FCC\_A1  
 Calculated 25 equilibria

Phase region boundary 12 at: 9.944E-01 1.100E+03  
 BCC\_A2  
 \*\* FCC\_A1  
 Calculated 16 equilibria

\*\*\* BUFFER SAVED ON FILE:  
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex01\BINA  
 RY.POLY3  
 CPU time for mapping 1 seconds

POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

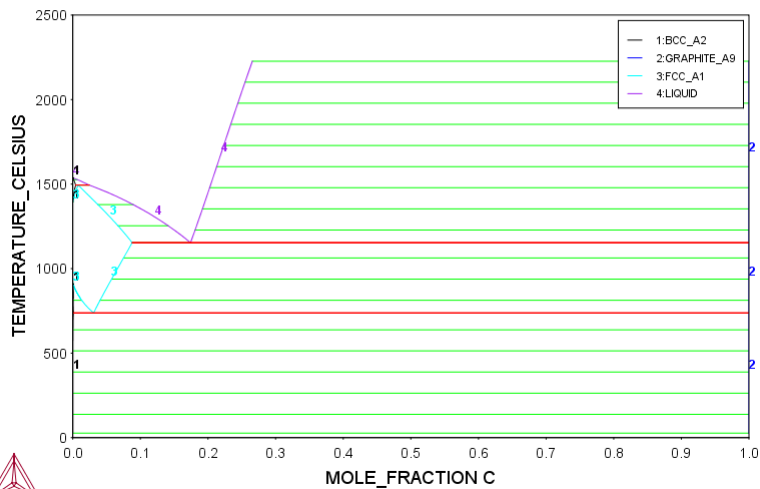
POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

... the command in full is SET\_TIELINE\_STATUS  
 ... the command in full is SET\_LABEL\_CURVE\_OPTION  
 ... the command in full is PLOT DIAGRAM

C FE

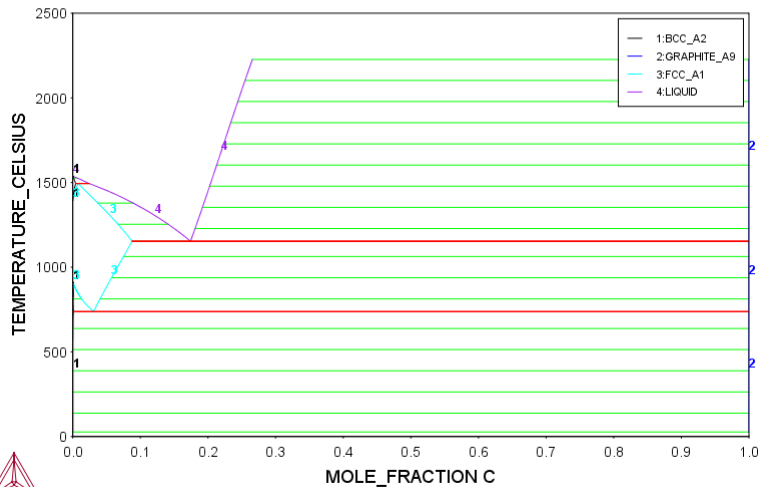
2016.05.16.12.58.24  
 TCBIN: C, FE  
 P=1E5, N=1



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

example 1a

2016.05.16.12.58.25  
 TCBIN: C, FE  
 P=1E5, N=1



POST:  
 POST:Hit RETURN to continue  
 POST: @@ By default no label is given, the user must specify it himself.  
 POST: @@ There are two possibilities, to label the lines or to label the  
 POST: @@ areas. In the latter case the user must supply a coordinate for the  
 POST: @@ label, for example  
 POST: ADD  
 ... the command in full is ADD\_LABEL\_TEXT  
 Give X coordinate in axis units: 1  
 Give Y coordinate in axis units: 2000  
 Automatic phase labels? /Y/: Y  
 Automatic labelling not always possible  
 Using global minimization procedure

Calculated 414 grid points in 0 s  
Found the set of lowest grid points in 0 s  
Calculated POLY solution 0 s, total time 0 s  
Stable phases are: LIQUID

Text size: /.36/:

POST: set-title example 1b

POST:

POST: plot

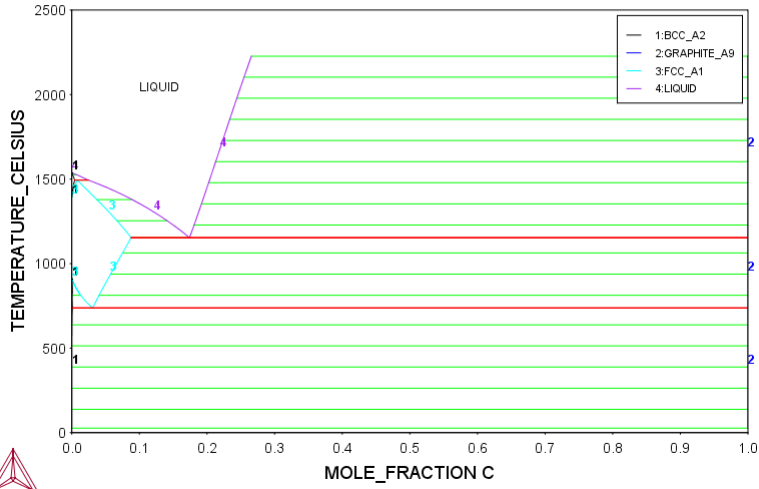
... the command in full is PLOT DIAGRAM

example 1b

2016.05.16.12.58.25

TCBIN: C, FE

P=1E5, N=1



POST:

POST:

POST:Hit RETURN to continue

POST: add .4 900

... the command in full is ADD\_LABEL\_TEXT

Automatic phase labels? /Y/: Y

Automatic labelling not always possible

Using global minimization procedure

Calculated 414 grid points in 0 s

Found the set of lowest grid points in 0 s

Calculated POLY solution 0 s, total time 0 s

Stable phases are: FCC\_A1+GRAPHITE\_A9

Text size: /.36/:

POST: set-title example 1c

POST:

POST: plot

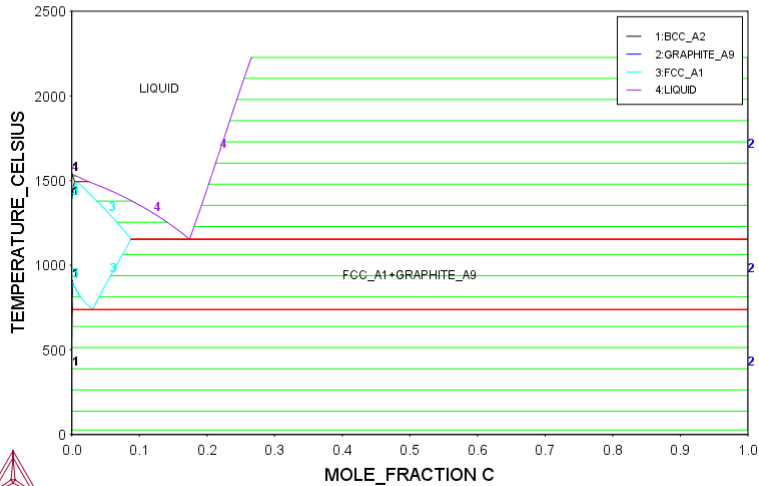
... the command in full is PLOT DIAGRAM

example 1c

2016.05.16.12.58.26

TCBIN: C, FE

P=1E5, N=1



POST:

POST:

POST:Hit RETURN to continue

POST: @@ This is the stable phase diagram with graphite and no cementite.

POST: @@ In TC all relevant data from the calculation of the diagram is saved

POST: @@ and it is possible to plot the same diagram using other thermodynamic

POST: @@ quantities, for example replace the carbon composition with its activity

POST: @@ Find out the commands in the post processor by inputting ?

POST: ?

... the command in full is HELP

ADD_LABEL_TEXT	PLOT_DIAGRAM	SET_INTERACTIVE_MODE
APPEND_EXPERIMENTAL_DATA	PRINT_DIAGRAM	SET_LABEL_CURVE_OPTION
BACK	QUICK_EXPERIMENTAL_PLOT	SET_PLOT_FORMAT
CHANGE_LEGEND	REINITIATE_PLOT_SETTINGS	SET_PLOT_OPTIONS
CREATE_3D_PLOTFILE	RESTORE_PHASE_IN_PLOT	SET_PLOT_SIZE
DUMP_DIAGRAM	SELECT_PLOT	SET_PREFIX_SCALING
ENTER_SYMBOL	SET_AXIS_LENGTH	SET_RASTER_STATUS
EXIT	SET_AXIS_PLOT_STATUS	SET_REFERENCE_STATE
FIND_LINE	SET_AXIS_TEXT_STATUS	SET_SCALING_STATUS
HELP	SET_AXIS_TYPE	SET_TIC_TYPE
LIST_DATA_TABLE	SET_COLOR	SET_TIELINE_STATUS
LIST_PLOT_SETTINGS	SET_CORNER_TEXT	SET_TITLE

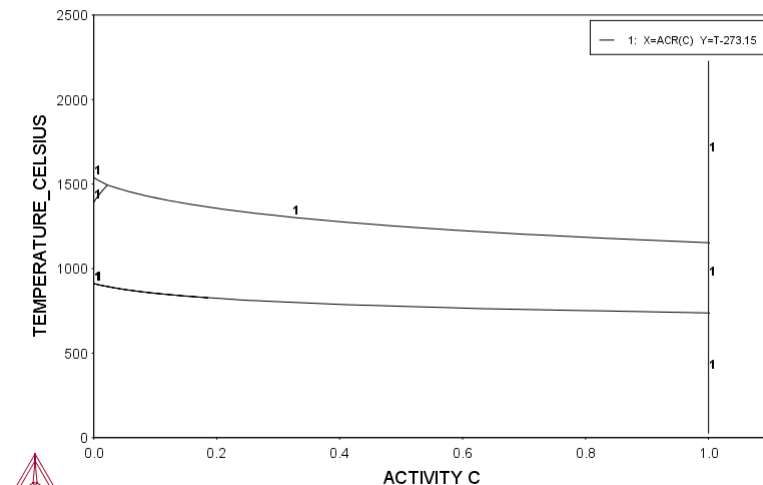
```

LIST_SYMBOLS          SET_DIAGRAM_AXIS          SET_TRUE_MANUAL_SCALING
MAKE_EXPERIMENTAL_DATAFI SET_DIAGRAM_TYPE      SUSPEND_PHASE_IN_PLOT
MODIFY_LABEL_TEXT     SET_FONT                 TABULATE
POST: @@ The command to set axis for the diagram is SET-DIAGRAM-AXIS
POST: s-d-a x
... the command in full is SET_DIAGRAM_AXIS
VARIABLE : ?
UNKNOWN QUESTION VARIABLE :
VARIABLE : ac
FOR COMPONENT : c
POST: set-title example 1d
POST:
POST: plot
... the command in full is PLOT DIAGRAM

```

**example 1d**

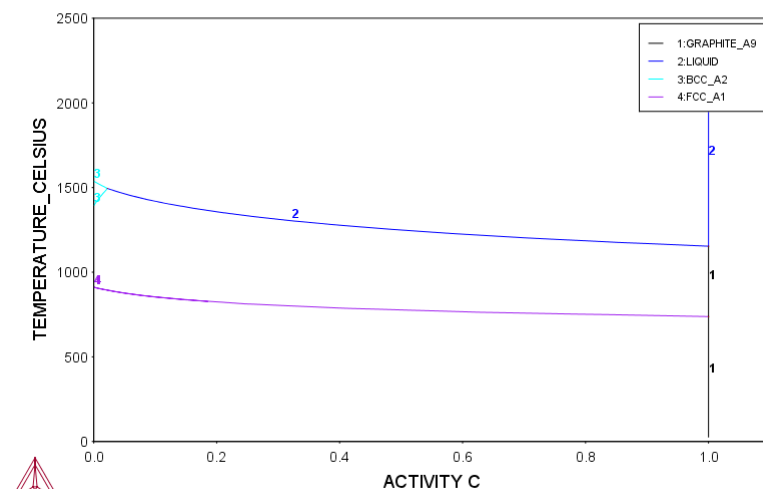
2016.05.16.12.58.26  
TCBIN: C, FE  
P=1E5, N=1



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

**example 1e**

2016.05.16.12.58.26  
TCBIN: C, FE  
P=1E5, N=1



POST:  
POST:  
POST:Hit RETURN to continue  
POST: @@ The metastable diagram, with cementite, can also be calculated but then  
POST: @@ one must do some manipulations in POLY. We can use the data  
POST: @@ we already retrieved from the database.  
POST: back  
Current database: Steels/Fe-Alloys v8.0

```

VA DEFINED
L12 FCC          B2_BCC          B2_VACANCY
HIGH_SIGMA      DICTRA_FCC_A1   REJECTED
SYS: go p-3
... the command in full is GOTO_MODULE
POLY_3:
POLY_3: @@ The BIN module has used the poly-3 workspace to calculate the
POLY_3: @@ diagram. We have all data available here. The workspace has been
POLY_3: @@ saved on a file and we can read this back with the command READ.
POLY_3:
POLY_3: read,,,
... the command in full is READ_WORKSPACES
POLY_3:
POLY_3: @@ There are many command in the POLY module. They make it possible
POLY_3: @@ to calculate almost any kind of equilibrium and diagram.
POLY_3: @@ With the ? we can list all commands
POLY_3: ?
... the command in full is HELP
ADD_INITIAL_EQUILIBRIUM  EXIT          REINITIATE_MODULE
ADVANCED_OPTIONS         GOTO_MODULE   SAVE_WORKSPACES
AMEND_STORED_EQUILIBRIA  HELP          SELECT_EQUILIBRIUM
BACK                     INFORMATION    SET_ALL_START_VALUES
CHANGE_STATUS            LIST_AXIS_VARIABLE SET_AXIS_VARIABLE
COMPUTE_EQUILIBRIUM      LIST_CONDITIONS SET_CONDITION
COMPUTE_TRANSITION       LIST_EQUILIBRIUM SET_INPUT_AMOUNTS
CREATE_NEW_EQUILIBRIUM   LIST_INITIAL_EQUILIBRIA SET_INTERACTIVE
DEFINE_COMPONENTS        LIST_STATUS   SET_NUMERICAL_LIMITS
DEFINE_DIAGRAM           LIST_SYMBOLS   SET_REFERENCE_STATE
DEFINE_MATERIAL           LOAD_INITIAL_EQUILIBRIUM SET_START_CONSTITUTION
DELETE_INITIAL_EQUILIB   MACRO_FILE_OPEN SET_START_VALUE
DELETE_SYMBOL            MAP           SHOW_VALUE
ENTER_SYMBOL            POST           STEP_WITH_OPTIONS
EVALUATE_FUNCTIONS       READ_WORKSPACES TABULATE
POLY_3:
POLY_3:Hit RETURN to continue
POLY_3: @@ More information about a command can be obtained with the HELP command
POLY_3: help
COMMAND: list-status

```

LIST\_STATUS

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

Synopsis 1: LIST\_STATUS <keyword(s)>  
Synopsis 2: LIST\_STATUS  
Ensuing Prompt: Option /CPS/: <keyword(s)>

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

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

The statuses of components, phases and species can be changed with the CHANGE\_STATUS command.

Results: Depending upon the key word specified in the CHANGE\_STATUS options, a table with the current statuses of phases or species or components, or their combinations, is shown up.

- \* For components, their statuses and reference states are listed.
- \* For ENTERED and FIXED phases, their statuses, driving forces and equilibrated amount (of stable) are listed. Note that the metastable phases are listed in descending order of stability. To avoid long outputs, in the versions later than version N, only 10 metastable phases (in ENTERED status) will be listed by lines, while all other less stable phases are merged onto one line. For DORMANT phases, their phase names and driving forces are listed. For SUSPENDED phases, only the phase names are listed into one line.
- \* For species, only the status are listed out.

Example:

```

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

```

The statuses of components, phases and species can be changed with the CHANGE\_STATUS command.

```

POLY_3:Hit RETURN to continue
POLY_3: @@ General information can be obtained using the INFORMATION command
POLY_3: INFO

```

... the command in full is INFORMATION  
WHICH SUBJECT /PURPOSE/:  
PURPOSE

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

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

With the comprehensive Equilibrium Calculation module, POLY ? it is possible to calculate many different kinds of equilibria and diagrams, in particular multicomponent phase diagrams. This is thus an important tool in developing new materials and processes. The current POLY module is its third version; this is why is often referred as POLY\_3 in the Thermo-Calc software.

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

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

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

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

- \* Direct Global Minimization: From the mesh of Gibbs energy, find the set of grid points that gives the lowest energy solution under the specified conditions. This set of grid points provides starting combination of phases and their constitutions for regular minimization to find the exact equilibrium solution. This solution will be then subject to a global test as described below.
- \* Indirect Global Minimization: Under certain conditions, direct approach is impossible. In this case, regular minimization is performed first and then a check is performed in order to see if the found local minimum is a global one by checking if all grid points are above the equilibrium Gibbs energy plane. If not, then recalculate by including these grid points until no grid point is above the equilibrium Gibbs energy plane from the previous step.

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

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

- \* The main cost in time comes from the calculation of Gibbs energy at each grid point generated by properly meshing the composition space for each entered phase. In a typical multicomponent system calculation, about 100MB of RAM memory is needed in storing the mesh of Gibbs energies.
- \* An additional (but much smaller) cost in time comes from finding the set of grid points in the above mesh that give the lowest energy solution. This solution is where POLY starts its ordinary minimization. When POLY has found an equilibrium, the equilibrium Gibbs energy surface is compared to the mesh to assure that no grid point is below the surface, i.e. a global minimization has been reached.

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

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

Together with the PARROT module, the POLY module is also used for critical assessment of experimental data in order to develop thermodynamic databases.

The POLY module uses the Gibbs Energy System (GES) for modeling and data manipulations of the thermodynamic properties of each phase.

The following commands are available in the POLY module:

```
POLY 3:?
ADD_INITIAL_EQUILIBRIUM  EXIT                REINITIATE_MODULE
ADVANCED_OPTIONS         GOTO_MODULE          SAVE_WORKSPACES
AMEND_STORED_EQUILIBRIA  HELP                SELECT_EQUILIBRIUM
BACK                     INFORMATION          SET_ALL_START_VALUES
CHANGE_STATUS            LIST_AXIS_VARIABLE  SET_AXIS_VARIABLE
COMPUTE_EQUILIBRIUM      LIST_CONDITIONS    SET_CONDITION
COMPUTE_TRANSITION       LIST_EQUILIBRIUM    SET_INPUT_AMOUNTS
CREATE_NEW_EQUILIBRIUM   LIST_INITIAL_EQUILIBRIA SET_INTERACTIVE
DEFINE_COMPONENTS        LIST_STATUS        SET_NUMERICAL_LIMITS
DEFINE_DIAGRAM           LIST_SYMBOLS        SET_REFERENCE_STATE
DEFINE_MATERIAL          LOAD_INITIAL_EQUILIBRIUM SET_START_CONSTITUTION
DELETE_INITIAL_EQUILIB   MACRO_FILE_OPEN    SET_START_VALUE
DELETE_SYMBOL            MAP                SHOW_VALUE
ENTER_SYMBOL             POST               STEP_WITH_OPTIONS
EVALUATE_FUNCTIONS       READ_WORKSPACES     TABULATE
POLY 3:
```

Note that, since TCCS, the SPECIAL\_OPTIONS and SET\_MINIMIZAION\_OPTIONS commands (the later one was introduced in the TCCR version) has been merged into the new ADVANCED\_OPTIONS command; and the RECOVER\_START\_VALUES command has been removed, due to that is not relevant to the POLY module anymore.

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

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

WHICH SUBJECT: ?

WHICH SUBJECT

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

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

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

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

WHICH SUBJECT: state

STATE VARIABLES

Standard State Variables and Partial Derivatives  
\*\*\*\*\*

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

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

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



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

Note that the Thermo-Calc software distinguishes between components of a system and constituent (i.e., species) of a phase in the system. Many state variables require one or the other. By default, the elements are defined as the system components, but this definition can be changed with the POLY command DEFINE\_COMPONENT. For instance, if the elements are Ca, Si and O, the another set of components can be defined as CaO, SiO and O<sub>2</sub>; in a pure water system, the components are normally defined as H<sub>2</sub>O and H<sup>+</sup>. However, one can not change the number of components when using this command.

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

The POLY module operates on a thermodynamic system in a stable or meta-stable or partial/local equilibrium state that is described by state variables. Examples of state variables are temperature, mole fraction, chemical potential and activity of a component (in the system or in a specific phase), enthalpy (of the system or a specific phase), etc. In the POLY module, a general notational method has been designed for the important set of standard state variables and their partial derivatives (or called as derived variables).

Common examples of state variables in a defined system are:

T	for temperature (K)
P	for pressure (Pa)
N	for total system size (in moles)
B	for total system site (in grams)
N(H)	for overall mole number of the hydrogen component
B(H <sub>2</sub> O)	for overall mass (grams) of the H <sub>2</sub> O component
X(Fe)	for overall mole fraction of the Fe component
W(AL <sub>2</sub> O <sub>3</sub> )	for overall mass fraction of the AL <sub>2</sub> O <sub>3</sub> component
Y(HCP,CR#1)	for site fraction of the Cr species on the first sublattice site in the HCP phase
X(LIQUID,Fe)	for mole fraction of the Fe component in the LIQUID phase
W(FCC,C)	for mass fraction of the C component in the FCC phase
NP(BCC)	for mole number of the BCC phase
BP(BCC)	for mass (grams) of the BCC phase
VP(BCC)	for volume (m <sup>3</sup> ) of the BCC phase
DGM(BCC)	for driving force of the BCC phase per mole of components
QF(SIGMA)	for phase stability function of the SIGMA phase
MUR(C)	for chemical potential of the C component (with regard to its reference state)
ACR(C)	for activity of the C component (with regard to its reference state)
LNACR(C)	for natural logarithm of activity of the C component [lnACR(C)=MUR(C)/RT]
MUR(Fe+3,AQ)	for chemical potential of the Fe+3 species related to the aqueous solution phase
ACR(Fe+3,AQ)	for activity of the Fe+3 species related to the aqueous solution phase
LNACR(Fe+3,AQ)	for natural logarithm of activity of the Fe+3 species related to the aqueous solution phase [lnACR(Fe+3,AQ)=MUR(Fe+3,AQ)/RT]
HM	for total enthalpy per mole component in the system
HM(FCC)	for enthalpy per mole component of the FCC phase
HM.T	for heat capacity per mole of components in the system (in J/mol/K)
HM(FCC).T	for heat capacity per mole of components of the FCC phase (in J/mol/K)
P.T	for the slope $\Delta P/\Delta T$ of a phase boundary on a P-T phase diagram. Note that the equilibrium with a phase assemblage must have been calculated.
T.W(Si)	for the slope $\Delta T/\Delta W(\text{Si})$ of a phase boundary on a T-W(Si) phase diagram with regard to mass of the component in the system
T.X(LIQ,CR)	for the slope $\Delta T/\Delta X(\text{LiQ,CR})$ of a phase boundary on a T-X(Liq,Cr) phase diagram with regard to mole fraction of the component in the phase

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

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

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

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

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

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

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

WHICH SUBJECT:  
POLY\_3:Hit RETURN to continue

```

POLY_3: @@ We can list the current equilibrium by
POLY_3: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: ?

OPTIONS

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

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

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

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

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

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

FCC_A1          Status ENTERED   Driving force  0.0000E+00
Moles 9.2463E-01, Mass 5.1201E+01, Volume fraction 0.0000E+00 Mass fractions:
FE 9.9766E-01 C 2.33819E-03

BCC_A2          Status ENTERED   Driving force  0.0000E+00
Moles 7.5373E-02, Mass 4.2079E+00, Volume fraction 0.0000E+00 Mass fractions:
FE 9.99907E-01 C 9.33835E-05
POLY_3:Hit RETURN to continue
POLY_3: @@ The actual conditions are listed by the list-equil command but
POLY_3: @@ can be obtained also by
POLY_3: l-c
... the command in full is LIST_CONDITIONS
X(FE)=0.99, P=1E5, N=1, T=1100
DEGREES OF FREEDOM 0
POLY_3:
POLY_3:Hit RETURN to continue
POLY_3: @@ The meaning of the state variables T, P, X, N and many others
POLY_3: @@ are explained by the INFO command
POLY_3: INFO
... the command in full is INFORMATION
WHICH SUBJECT /PURPOSE/: state
STATE VARIABLES

Standard State Variables and Partial Derivatives
*****

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

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

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

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

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

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

The POLY module operates on a thermodynamic system in a stable or meta-stable
or partial/local equilibrium state that is described by state variables.
Examples of state variables are temperature, mole fraction, chemical
potential and activity of a component (in the system or in a specific
phase), enthalpy (of the system or a specific phase), etc. In the POLY
module, a general notational method has been designed for the important
set of standard state variables and their partial derivatives (or called

```

as derived variables).

Common examples of state variables in a defined system are:

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

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

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

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

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

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

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

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

#### WHICH SUBJECT:

POLY\_3:Hit RETURN to continue

POLY\_3: @@ The use of state variables as conditions is the key to the

POLY\_3: @@ flexibility of TC. Each condition is set independently and

POLY\_3: @@ any condition can be set as axis variable.

POLY\_3: @@

POLY\_3: @@ Now we just want to take away the graphite in order to calculate the

POLY\_3: @@ metastable Fe-C diagram with cementite. We can list all phases by the

POLY\_3: @@ LIST\_STATUS command

POLY\_3: l-st

... the command in full is LIST\_STATUS

#### Option /CPS/:

*** STATUS FOR ALL COMPONENTS					
COMPONENT	STATUS	REF. STATE	T(K)	P(Pa)	
VA	ENTERED	SER			
C	ENTERED	GRAPHITE_A9	*	100000	
FE	ENTERED	BCC_A2	*	100000	
*** STATUS FOR ALL PHASES					
PHASE	STATUS	DRIVING FORCE	MOLES		
FCC_A1	ENTERED	0.000000E+00	9.246266E-01		
BCC_A2	ENTERED	0.000000E+00	7.537335E-02		
D011_CEMENTITE	ENTERED	-4.153716E-01	0.000000E+00		
LIQUID	ENTERED	-4.668963E-01	0.000000E+00		
GRAPHITE_A9	ENTERED	-1.684424E+00	0.000000E+00		
DIAMOND_A4	ENTERED	-2.386932E+00	0.000000E+00		
*** STATUS FOR ALL SPECIES					
C	ENTERED	C3	ENTERED	FE	ENTERED VA ENTERED

```
C1 ENTERED C4 ENTERED FE+2 ENTERED VA-2 ENTERED
C2 ENTERED C5 ENTERED FE+3 ENTERED VA-4 ENTERED
```

POLY\_3:Hit RETURN to continue

POLY\_3: @@ The status is changed by the CHANGE\_STATUS command

POLY\_3: ch-st

... the command in full is CHANGE\_STATUS

For phases, species or components? /PHASES/:

Phase name(s): ?

Phase name(s)

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

Phase name(s): gra

Status: /ENTERED/: sus

POLY\_3: l-st

... the command in full is LIST\_STATUS

Option /CPS/:

\*\*\* STATUS FOR ALL COMPONENTS

COMPONENT	STATUS	REF. STATE	T(K)	P(Pa)
VA	ENTERED	SER		
C	ENTERED	GRAPHITE_A9	*	100000
FE	ENTERED	BCC_A2	*	100000

\*\*\* STATUS FOR ALL PHASES

PHASE	STATUS	DRIVING FORCE	MOLES
FCC_A1	ENTERED	0.000000E+00	9.246266E-01
BCC_A2	ENTERED	0.000000E+00	7.537335E-02
D011_CEMENTITE	ENTERED	-4.153716E-01	0.000000E+00
LIQUID	ENTERED	-4.668963E-01	0.000000E+00
DIAMOND_A4	ENTERED	-2.386932E+00	0.000000E+00

SUSPENDED PHASES:

GRAPHITE\_A9

\*\*\* STATUS FOR ALL SPECIES

C	ENTERED	C3	ENTERED	FE	ENTERED	VA	ENTERED
C1	ENTERED	C4	ENTERED	FE+2	ENTERED	VA-2	ENTERED
C2	ENTERED	C5	ENTERED	FE+3	ENTERED	VA-4	ENTERED

POLY\_3:Hit RETURN to continue

POLY\_3: @@ Note that the graphite is listed as suspended this time.

POLY\_3: @@ we try to calculate the equilibrium without graphite.

POLY\_3: c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Using global minimization procedure

Calculated 413 grid points in 0 s

Found the set of lowest grid points in 0 s

Calculated POLY solution 0 s, total time 0 s

POLY\_3: @@ A number of ,, after a command means to accept default values.

POLY\_3: l-e,,,

... the command in full is LIST\_EQUILIBRIUM

Output from POLY-3, equilibrium = 1, label A0, database: TCBIN

Conditions:

X(FE)=0.99, P=1E5, N=1, T=1100

DEGREES OF FREEDOM 0

Temperature 1100.00 K ( 826.85 C), Pressure 1.000000E+05

Number of moles of components 1.00000E+00, Mass in grams 5.54086E+01

Total Gibbs energy -4.90502E+04, Enthalpy 3.18534E+04, Volume 0.00000E+00

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

FCC\_A1 Status ENTERED Driving force 0.0000E+00

Moles 9.2463E-01, Mass 5.1201E+01, Volume fraction 0.0000E+00 Mass fractions:

FE 9.97662E-01 C 2.33819E-03

BCC\_A2 Status ENTERED Driving force 0.0000E+00

Moles 7.5373E-02, Mass 4.2079E+00, Volume fraction 0.0000E+00 Mass fractions:

FE 9.99907E-01 C 9.33835E-05

POLY\_3:Hit RETURN to continue

POLY\_3: @@ It may seem surprising that diamond is stable but the total mole fraction

POLY\_3: @@ of iron is less than 0.5, so we are on the carbon rich side

POLY\_3: @@ of cementite, and it is reasonable.

POLY\_3:

POLY\_3: @@ Now try to map the metastable diagram now

POLY\_3: map

Version S mapping is selected

Generating start equilibrium 1

Generating start equilibrium 2

Generating start equilibrium 3

Generating start equilibrium 4

Generating start equilibrium 5

Generating start equilibrium 6

Generating start equilibrium 7

Generating start equilibrium 8

Generating start equilibrium 9

Generating start equilibrium 10

Generating start equilibrium 11

Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1

Generating start point 2

Generating start point 3

Generating start point 4

Generating start point 5

Generating start point 6

Generating start point 7

Generating start point 8

Generating start point 9

Generating start point 10

Working hard

Generating start point 11

Generating start point 12

```

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Phase region boundary 18 at: 5.000E-01 3.100E+02
  BCC_A2
  ** DIAMOND_A4
Calculated.. 2 equilibria

```

Terminating at known equilibrium  
Terminating at axis limit.

Phase region boundary 19 at: 5.000E-01 3.100E+02  
BCC\_A2  
\*\* DIAMOND\_A4  
Calculated. 24 equilibria  
Terminating at known equilibrium

Phase region boundary 20 at: 5.000E-01 3.100E+02  
BCC\_A2  
\*\* DIAMOND\_A4  
Calculated.. 2 equilibria  
Terminating at known equilibrium  
Terminating at axis limit.

Phase region boundary 21 at: 5.000E-01 3.100E+02  
BCC\_A2  
\*\* DIAMOND\_A4  
Calculated. 24 equilibria  
Terminating at known equilibrium

Phase region boundary 22 at: 5.000E-01 3.100E+02  
BCC\_A2  
\*\* DIAMOND\_A4  
Calculated.. 2 equilibria  
Terminating at known equilibrium  
Terminating at axis limit.

Phase region boundary 23 at: 5.000E-01 3.100E+02  
BCC\_A2  
\*\* DIAMOND\_A4  
Calculated. 24 equilibria  
Terminating at known equilibrium

Phase region boundary 24 at: 5.000E-01 3.100E+02  
BCC\_A2  
\*\* DIAMOND\_A4  
Calculated.. 2 equilibria  
Terminating at known equilibrium  
Terminating at axis limit.

Phase region boundary 25 at: 5.000E-01 3.100E+02  
BCC\_A2  
\*\* DIAMOND\_A4  
Calculated. 24 equilibria  
Terminating at known equilibrium

Phase region boundary 26 at: 5.000E-01 3.100E+02  
BCC\_A2  
\*\* DIAMOND\_A4  
Calculated.. 2 equilibria  
Terminating at known equilibrium  
Terminating at axis limit.

Phase region boundary 27 at: 5.000E-01 3.100E+02  
BCC\_A2  
\*\* DIAMOND\_A4  
Calculated. 24 equilibria  
Terminating at known equilibrium

Phase region boundary 28 at: 3.750E-01 1.037E+03  
\*\* D011\_CEMENTITE  
DIAMOND\_A4  
Calculated. 9 equilibria  
Terminating at known equilibrium

Phase region boundary 29 at: 3.750E-01 1.037E+03  
\*\* D011\_CEMENTITE  
DIAMOND\_A4  
Calculated. 19 equilibria  
Terminating at known equilibrium

Phase region boundary 30 at: 9.877E-01 1.037E+03  
BCC\_A2  
\*\* FCC\_A1  
Calculated. 3 equilibria  
Terminating at known equilibrium

Phase region boundary 31 at: 9.877E-01 1.037E+03  
BCC\_A2  
\*\* FCC\_A1  
Calculated 23 equilibria

Phase region boundary 32 at: 3.754E-01 1.763E+03  
LIQUID  
\*\* DIAMOND\_A4  
Calculated. 13 equilibria  
Terminating at known equilibrium

Phase region boundary 33 at: 3.754E-01 1.763E+03  
LIQUID  
\*\* DIAMOND\_A4  
Calculated.. 31 equilibria  
Terminating at known equilibrium  
Terminating at axis limit.

Phase region boundary 34 at: 9.820E-01 1.763E+03  
LIQUID  
\*\* FCC\_A1  
Calculated. 15 equilibria  
Terminating at known equilibrium

Phase region boundary 35 at: 9.820E-01 1.763E+03  
LIQUID  
\*\* FCC\_A1  
Calculated. 2 equilibria  
Terminating at known equilibrium

Phase region boundary 36 at: 3.306E-01 2.490E+03  
LIQUID  
\*\* DIAMOND\_A4  
Calculated. 42 equilibria  
Terminating at known equilibrium

Phase region boundary 37 at: 3.306E-01 2.490E+03

```

    LIQUID
    ** DIAMOND_A4
    Calculated..                2 equilibria
    Terminating at known equilibrium
    Terminating at axis limit.

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

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

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

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

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

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

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

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

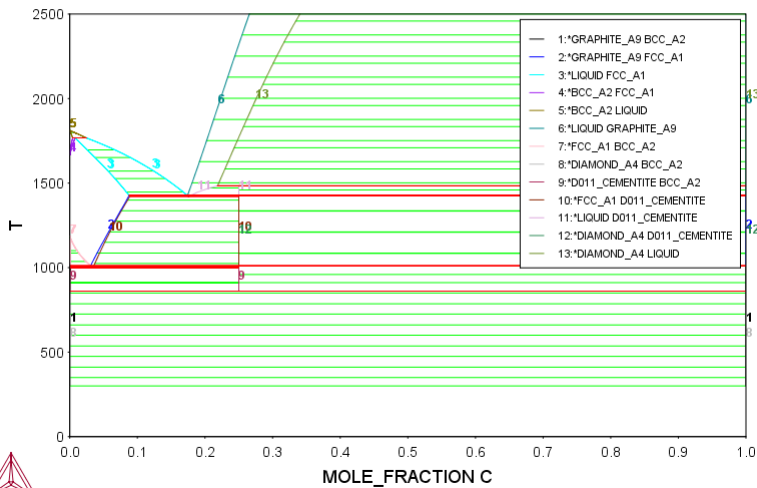
Phase region boundary 46 at: 9.941E-01 1.794E+03
    LIQUID
    ** BCC_A2
    Calculated..                2 equilibria
    Terminating at known equilibrium

Phase region boundary 47 at: 9.941E-01 1.794E+03
    LIQUID
    ** BCC_A2
    Calculated..                12 equilibria
    *** BUFFER SAVED ON FILE:
    c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex01\BINA
    RY.POLY3
    CPU time for mapping                1 seconds
POLY_3:
POLY_3: post
POST: s-d-a y t
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a x m-f C
... the command in full is SET_DIAGRAM_AXIS
POST: set-tieline
... the command in full is SET_TIELINE_STATUS
PLOTting EVERY TIE-LINE NO /5/: 5
POST:
POST: set-title example 1f
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

# example 1f

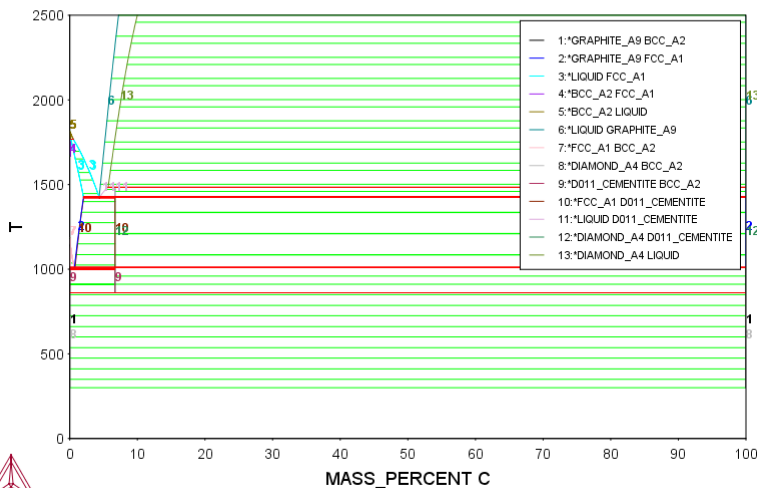
2016.05.16.12.58.32  
TCBIN: C, FE  
P=1E5, N=1



POST:  
POST:  
POST:Hit RETURN to continue  
POST: @@ The previous stable diagram is also plotted. The reason is that  
POST: @@ we never removed it from the workspace (It can be done with a SAVE  
POST: @@ command, please read about this command).  
POST: @@  
POST: @@ It may be surprising to find that diamond is more stable than  
POST: @@ cementite at low temperature. However, one would never find  
POST: @@ diamonds in steel, unfortunately, as graphite would form first.  
POST: @@  
POST: @@ Now change the axis to composition, use weight-percent of carbon  
POST: s-d-a x  
... the command in full is SET\_DIAGRAM\_AXIS  
VARIABLE : ?  
UNKNOWN QUESTION VARIABLE :  
VARIABLE : w-p  
FOR COMPONENT : c  
POST: set-title example 1g  
POST:  
POST: plot  
... the command in full is PLOT DIAGRAM

# example 1g

2016.05.16.12.58.32  
TCBIN: C, FE  
P=1E5, N=1



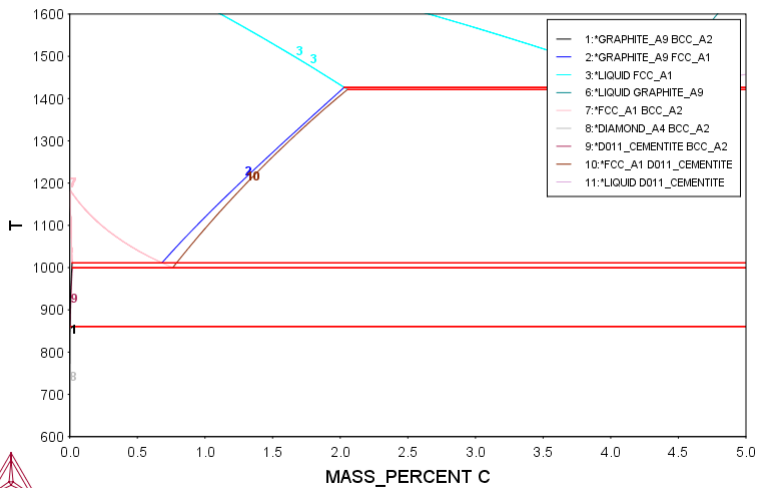
POST:  
POST:  
POST:Hit RETURN to continue  
POST: @@ The tie-lines now obscure the diagram, take them away  
POST: @@ Also change the scale of the x and y axis  
POST: s-t-s 0  
... the command in full is SET\_TIELINE\_STATUS  
POST: s-s x n 0 5  
... the command in full is SET\_SCALING\_STATUS  
POST: s-s y n 600 1600  
... the command in full is SET\_SCALING\_STATUS  
POST: set-title example 1h  
POST:  
POST: plot  
... the command in full is PLOT\_DIAGRAM



5

## example 1h

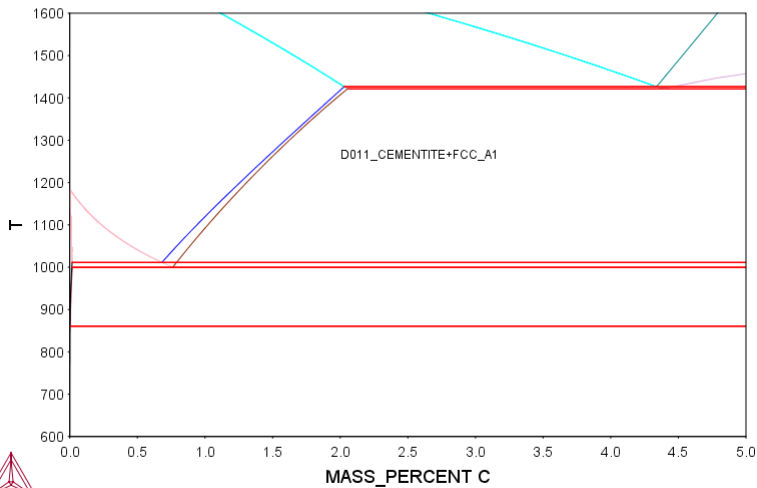
2016.05.16.12.58.32  
TCBIN: C, FE  
P=1E5, N=1 4



POST:  
POST:  
POST:Hit RETURN to continue  
POST: @@ Finally add some nice labels  
POST: set-lab n  
... the command in full is SET\_LABEL\_CURVE\_OPTION  
POST: add 2 1250  
... the command in full is ADD\_LABEL\_TEXT  
Automatic phase labels? /Y/:  
Automatic labelling not always possible  
Using global minimization procedure  
Calculated 413 grid points in 0 s  
Found the set of lowest grid points in 0 s  
Calculated POLY solution 0 s, total time 0 s  
Stable phases are: D011\_CEMENTITE+FCC\_A1  
Text size: /.36/:  
POST: set-title example 1i  
POST:  
POST: plot  
... the command in full is PLOT DIAGRAM

## example 1i

2016.05.16.12.58.33  
TCBIN: C, FE  
P=1E5, N=1



POST:  
POST:  
POST:Hit RETURN to continue  
POST: add 1.5 900  
... the command in full is ADD\_LABEL\_TEXT  
Automatic phase labels? /Y/:  
Automatic labelling not always possible  
Using global minimization procedure  
Calculated 413 grid points in 0 s  
Found the set of lowest grid points in 0 s  
Calculated POLY solution 0 s, total time 0 s  
Stable phases are: BCC\_A2+D011\_CEMENTITE  
Text size: /.36/:  
POST: add 1.5 700  
... the command in full is ADD\_LABEL\_TEXT  
Automatic phase labels? /Y/:  
Automatic labelling not always possible  
Using global minimization procedure  
Calculated 413 grid points in 0 s  
Found the set of lowest grid points in 0 s  
Calculated POLY solution 0 s, total time 0 s  
Stable phases are: BCC\_A2+DIAMOND\_A4  
Text size: /.36/:  
POST: add .2 1500  
... the command in full is ADD\_LABEL\_TEXT  
Automatic phase labels? /Y/:  
Automatic labelling not always possible  
Using global minimization procedure

Calculated 413 grid points in 0 s  
 Found the set of lowest grid points in 0 s  
 Calculated POLY solution 0 s, total time 0 s  
 Stable phases are: FCC\_A1

Text size: /.36/:

POST: set-title example 1j

POST:

POST: plot

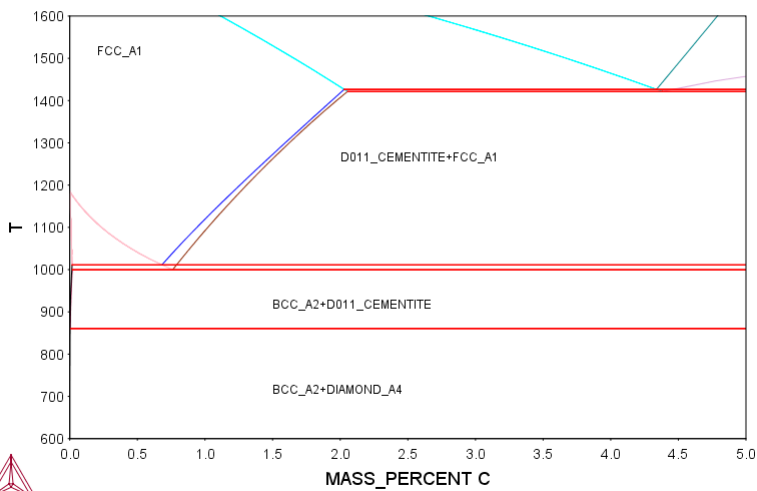
... the command in full is PLOT DIAGRAM

example 1j

2016.05.16.12.58.33

TCBIN: C, FE

P=1E5, N=1



POST:

POST:

POST: Hit RETURN to continue

POST: @@ As graphite is suspended cementite is the stable carbide

POST: @@ so that is the phase that will be listed in the two-phase regions.

POST: @@ The label for the FCC region is a bit too high, move it down

POST: modify

... the command in full is MODIFY\_LABEL\_TEXT

These labels are defined

No 1 at 2.00000E+00 1.25000E+03 : D011\_CEMENTITE+FCC\_A1

No 2 at 1.50000E+00 9.00000E+02 : BCC\_A2+D011\_CEMENTITE

No 3 at 1.50000E+00 7.00000E+02 : BCC\_A2+DIAMOND\_A4

No 4 at 2.00000E-01 1.50000E+03 : FCC\_A1

Which label to modify? /4/:

New X coordinate /.2/ : .2

New Y coordinate /1500/ : 1300

New text /FCC\_A1/:

POST: set-title example 1k

POST:

POST: plot

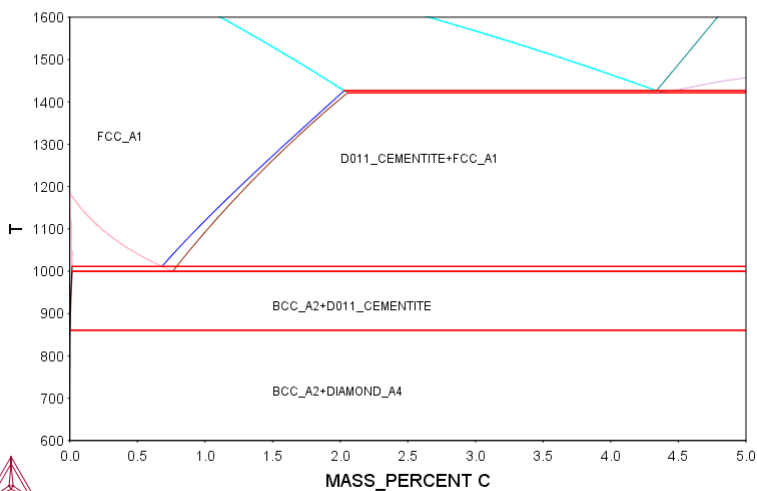
... the command in full is PLOT DIAGRAM

example 1k

2016.05.16.12.58.34

TCBIN: C, FE

P=1E5, N=1



POST:

POST: set-inter

... the command in full is SET\_INTERACTIVE\_MODE

POST:

tcex02

```
AboutMACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex02\tcex02.TCM"SYS:SYS:SYS:SYS:SYS:
SYS:
SYS:SYS:SYS: SET-ECHO
SYS: set-log ex02,,
SYS:
SYS:
SYS: go da
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
L12_FCC B2_BCC B2_VACANCY
HIGH_SIGMA DICTRA_FCC_A1 REJECTED
TDB_TCFE8: sw ssol5
... the command in full is SWITCH_DATABASE
Current database: SGTE Alloy Solutions Database v5.0

VA DEFINED
GAS:G REJECTED
TDB_SSOL5: @@ Pure Fe is selected as unary system
TDB_SSOL5: d-sys fe
... the command in full is DEFINE_SYSTEM
FE DEFINED
TDB_SSOL5: get
... the command in full is GET_DATA
REINITIATING GES5 .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
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... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

'Benyan Pei, B Bjorkman, B Sundman, and B Jansson: Calphad, 1995, 19(1), 1
-15. "A thermodynamic assessment of the Iron-Antimony system". >> Fe
-Sb '
'G Reumont, P Perrot, JM Fiorani, and J Hertz: J. Phase Equil.,, 2000, 21,
371-378. "Thermodynamic assessment of the Fe-Zn system". >> Fe-Zn '
-OK-
TDB_SSOL5:
TDB_SSOL5: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3: @@ In POLY-3 we first define a single equilibrium
POLY_3: s-c t=300,p=1e5,n=1
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 24 grid points in 0 s
POLY_3: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: SSOL5

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

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

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

BCC_B2 DISORD Status ENTERED Driving force 0.0000E+00
Moles 1.0000E+00, Mass 5.5847E+01, Volume fraction 0.0000E+00 Mass fractions:
FE 1.00000E+00
POLY_3:
POLY_3:Hit RETURN to continue
POLY_3: @@ We set T as axis variable
POLY_3: s-a-v
... the command in full is SET_AXIS_VARIABLE
Axis number: /1/: 1
Condition /NONE/: t
Min value /0/: 300
Max value /1/: 2000
Increment /42.5/: 42.5
POLY_3: @@ We always save in order to be able to come back to this point
POLY_3: save tcex02a y
... the command in full is SAVE_WORKSPACES
POLY_3: @@ Step along the axis
POLY_3: step
... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: NORMAL
No initial equilibrium, using default
Step will start from axis value 300.000
...OK

Phase Region from 300.000 for:
BCC_B2
Global test at 3.80000E+02 .... OK
Global test at 4.80000E+02 .... OK
Global test at 5.80000E+02 .... OK
Global test at 6.80000E+02 .... OK
Global test at 7.80000E+02 .... OK
Global test at 8.80000E+02 .... OK
```

```

Global test at 9.80000E+02 .... OK
Global test at 1.08000E+03 .... OK
Global test at 1.18000E+03 .... OK
Global check of adding phase at 1.18481E+03
Calculated 91 equilibria

Phase Region from 1184.81 for:
  BCC_B2
  FCC_L12
Calculated 2 equilibria

Phase Region from 1184.81 for:
  FCC_L12
Global Test at 1.26000E+03 .... OK
Global test at 1.36000E+03 .... OK
Global test at 1.46000E+03 .... OK
Global test at 1.56000E+03 .... OK
Global test at 1.66000E+03 .... OK
Global check of adding phase at 1.66747E+03
Calculated 51 equilibria

Phase Region from 1667.47 for:
  BCC_B2
  FCC_L12
Calculated 2 equilibria

Phase Region from 1667.47 for:
  BCC_B2
Global test at 1.74000E+03 .... OK
Global check of adding phase at 1.81095E+03
Calculated 18 equilibria

Phase Region from 1810.95 for:
  LIQUID
  BCC_B2
Calculated 2 equilibria

Phase Region from 1810.95 for:
  LIQUID
Global test at 1.89000E+03 .... OK
Global test at 1.99000E+03 .... OK
Terminating at 2000.00
Calculated 22 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex02\tcex
02a.POLY3
POLY_3: @@ Post processing is the essential part of this example
POLY_3: @@ We will plot Gm, Hm and Cp for some phases
POLY_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

```

Setting automatic diagram axes

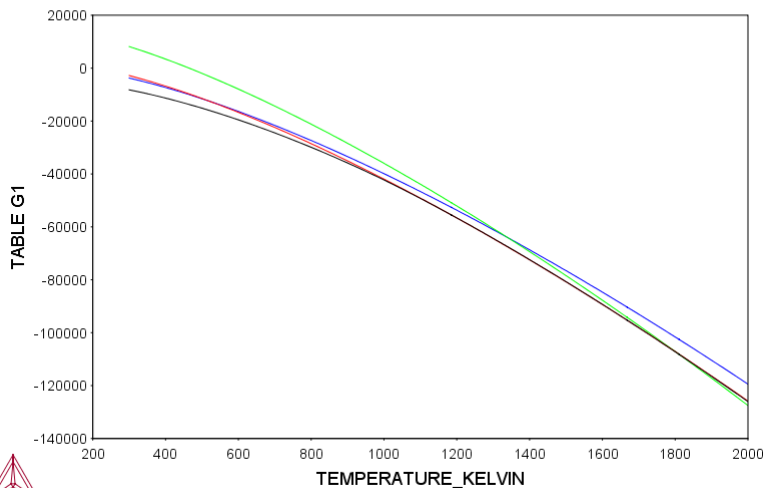
```

POST:
POST:
POST: @@ The x-axis will be the temperature in Kelvin
POST: s-d-a x
... the command in full is SET_DIAGRAM_AXIS
VARIABLE : ?
UNKNOWN QUESTION VARIABLE :
VARIABLE : t-k
POST: @@ The phases for which Gm shall be plotted must be defined
POST: @@ in a table
POST: ent tab
... the command in full is ENTER_SYMBOL
Name: g1
Variable(s): gm(bcc_b2) gm(fcc_l12) gm(liq) gm(hcp_a3)
&
POST:
POST: @@ The table is set as y-axis and all columns included
POST: s-d-a y g1
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: set-title example 2a
POST: plot
... the command in full is PLOT DIAGRAM

```

example 2a

2016.05.16.13.00.42  
SSOL5: FE  
P=1E5, N=1



```

POST:
POST: Hit RETURN to continue
POST: @@

```

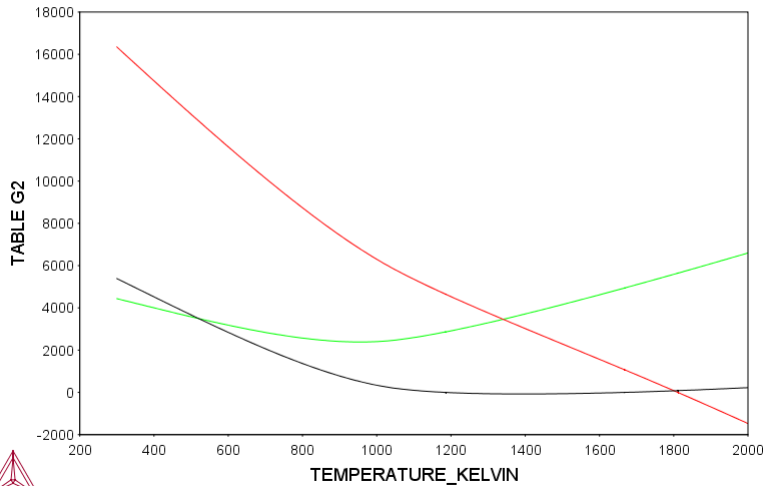
```

POST:
POST:
POST: @@ The magnitude makes it difficult to see anything. Enter
POST: @@ functions for the differences with respect to bcc
POST: ent fun dgf=gm(fcc_l12)-gm(bcc_b2);
... the command in full is ENTER_SYMBOL
POST: ent fun dgl=gm(liq)-gm(bcc_b2);
... the command in full is ENTER_SYMBOL
POST: ent fun dgh=gm(hcp_a3)-gm(bcc_b2);
... the command in full is ENTER_SYMBOL
POST: @@ and enter a new table and set it as y-axis
POST: ent tab g2
... the command in full is ENTER_SYMBOL
Variable(s): dgf dgl dgh;
POST: s-d-a y g2
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: set-title example 2b
POST:
POST: plot
... the command in full is PLOT DIAGRAM

```

example 2b

2016.05.16.13.00.42  
SSOL5: FE  
P=1E5, N=1



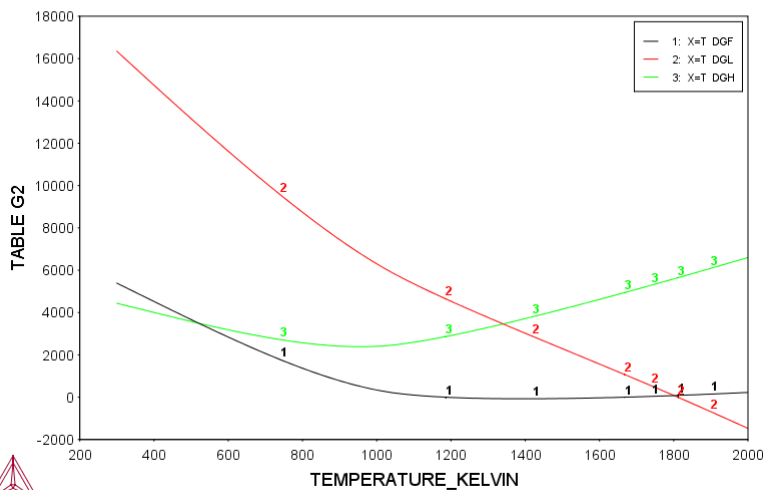
```

POST:
POST: Hit RETURN to continue
POST: @@ In order to have some identification on the lines
POST: @@ use the command SET_LABEL
POST: s-lab
... the command in full is SET_LABEL_CURVE_OPTION
CURVE LABEL OPTION (A, B, C, D, E, F OR N) /N/: D
POST: set-title example 2c
POST:
POST: plot
... the command in full is PLOT DIAGRAM

```

example 2c

2016.05.16.13.00.43  
SSOL5: FE  
P=1E5, N=1



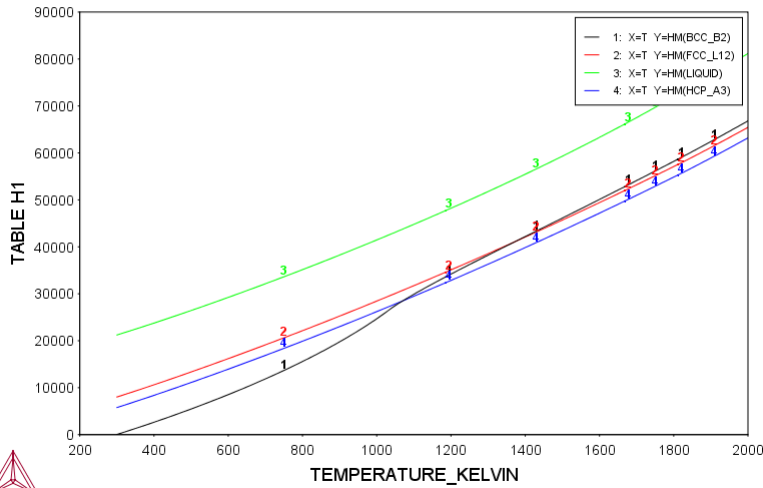
```

POST:
POST: Hit RETURN to continue
POST: @@ Now plot enthalpies
POST: ent tab h1
... the command in full is ENTER_SYMBOL
Variable(s): hm(bcc_b2) hm(fcc_l12) hm(liq) hm(hcp_a3);
POST: s-d-a y h1
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: set-title example 2d
POST:
POST: plot
... the command in full is PLOT DIAGRAM

```

# example 2d

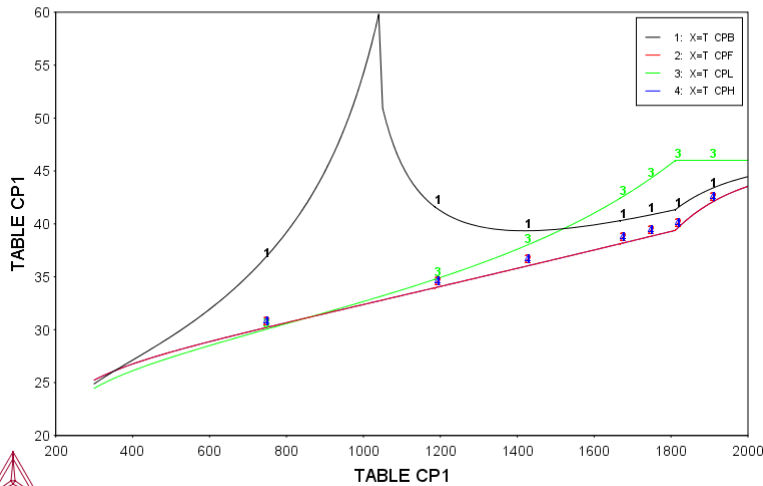
2016.05.16.13.00.43  
SSOL5: FE  
P=1E5, N=1



```
POST:
POST:Hit RETURN to continue
POST: @@ And finally plot heat capacities
POST: ent fun cpb=hm(bcc_b2).t;
... the command in full is ENTER_SYMBOL
POST: ent fun cpf=hm(fcc_l12).t;
... the command in full is ENTER_SYMBOL
POST: ent fun cpl=hm(liq).t;
... the command in full is ENTER_SYMBOL
POST: ent fun cph=hm(hcp_a3).t;
... the command in full is ENTER_SYMBOL
POST: ent tab cp1
... the command in full is ENTER_SYMBOL
Variable(s): t cpb cpf cpl cph;
POST: s-d-a y
... the command in full is SET_DIAGRAM_AXIS
VARIABLE : cp1
COLUMN NUMBER /*/: 2-5
POST: s-d-a x cp1 1
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 2e
POST:
POST: plot
... the command in full is PLOT DIAGRAM
```

# example 2e

2016.05.16.13.00.43  
SSOL5: FE  
P=1E5, N=1



```
POST:
POST:Hit RETURN to continue
POST: @@
POST: @@ In the next case plot functions for a binary system
POST: @@
POST: ba
... the command in full is BACK
POLY_3: go da
... the command in full is GOTO_MODULE
TDB_SSOL5: rej sys
... the command in full is REJECT
VA DEFINED
GAS:G REJECTED
REINITIATING GES5 .....
TDB_SSOL5: @@ select the Cu-Fe system and only
TDB_SSOL5: @@ the fcc, bcc, liquid and hcp phases
TDB_SSOL5: d-sys fe cu
... the command in full is DEFINE_SYSTEM
FE CU DEFINED
TDB_SSOL5: rej ph /all
... the command in full is REJECT
LIQUID:L FCC_A1 FCC_L12
FCC_DIS FCC_ORD BCC_A2
BCC_B2 HCP_A3 HCP_ZN
```

```

TETRAGONAL_U          CBCC_A12          CUB_A13
ORTHORHOMBIC_A20      LAVES_C14          LAVES_C15
LAVES_C36             M4N              ALCU_ETA
ALCU_EPSILON          ALCUZN_GAMMA_H      AL5FE4
CUSN_GAMMA_DO3        CUTI              CU4TI
CU6Y                  CUZN_GAMMA      D_GAMMA
FEPD                  FEPD3            FESB
FEU6                  FE2U            FEZN_GAMMA_D82
FEZN4                 FEZN_DELTA      FEZN_ZETA
FEUZR_DELTA           FEZR2            FEZR3
REJECTED
TDB_SSOL5: rest ph fcc_a1 bcc_a2 liq hcp_a3
... the command in full is RESTORE
FCC_A1                BCC_A2              LIQUID:L
HCP_A3 RESTORED
TDB_SSOL5: l-sys
... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/: CONSTITUENT
LIQUID:L              :CU FE:
FCC_A1                :CU FE:VA:
BCC_A2                :CU FE:VA:
HCP_A3                :CU FE:VA:
TDB_SSOL5: get
... the command in full is GET_DATA
REINITIATING GES5 .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ...

List of references for assessed data

'Data for the Cu-Fe system are from an unpublished assessment of I Ansara
and A Jansson published in the COST507 final report: COST507
Thermochemical Database for Light Metal Alloys, Vol 2, eds by I Ansara,
AT Dinsdale and MH Rand, July 1998, EUR18499. The data were also
reported by A Jansson in the KTH report TRITA-MAC-533, 1993. >> Cu-Fe '
-OK-
TDB_SSOL5: go p-3
... the command in full is GOTO_MODULE

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

Phase Region from 0.529789 for:
LIQUID
BCC_A2
FCC_A1
HCP_A3

Phase Region from 0.529789 for:
LIQUID
BCC_A2
FCC_A1
HCP_A3
*** Buffer saved on file ***
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex02\tcex
02b.POLY3
POLY_3: @@ Now plot the results in various ways
POLY_3: post

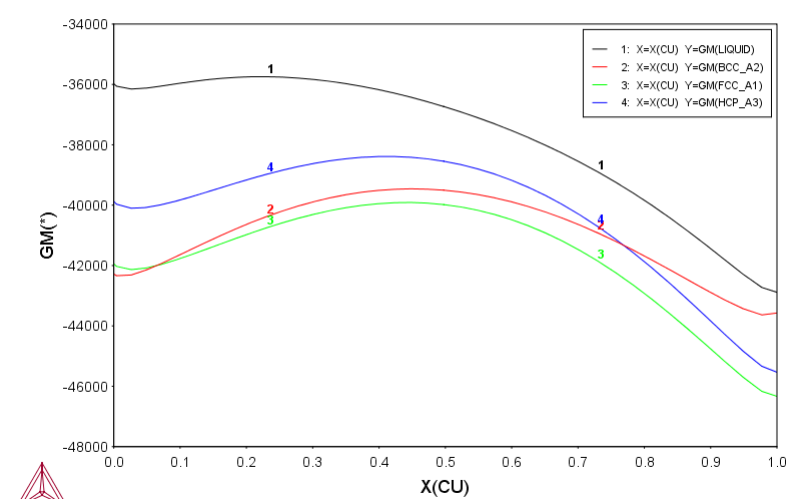
POLY-3 POSTPROCESSOR VERSION 3.2

POST: @@ Set the Gm of all phases on the y-axis
POST: s-d-a y gm(*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: @@ and the mole percent of Cu on the x-axis
POST: s-d-a x x(cu)
... the command in full is SET_DIAGRAM_AXIS
POST: set-lab d
... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: set-title example 2f
POST:

```

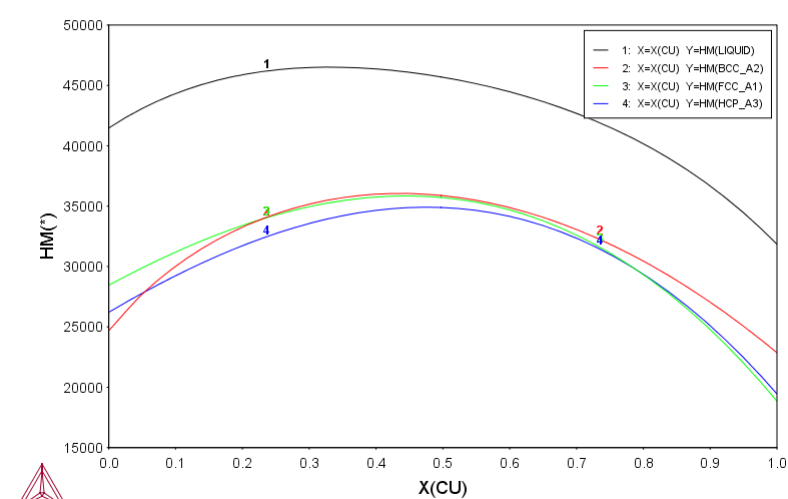
POST: plot  
... the command in full is PLOT DIAGRAM  
example 2f

2016.05.16.13.00.46  
SSOL5: CU, FE  
T=1000, P=1E5, N=1



POST:  
POST:Hit RETURN to continue  
POST: @@ Now plot the enthalpy  
POST: s-d-a y hm(\*)  
... the command in full is SET\_DIAGRAM\_AXIS  
COLUMN NUMBER /\*/: \*  
POST: set-title example 2g  
POST:  
POST: plot  
... the command in full is PLOT DIAGRAM  
example 2g

2016.05.16.13.00.47  
SSOL5: CU, FE  
T=1000, P=1E5, N=1

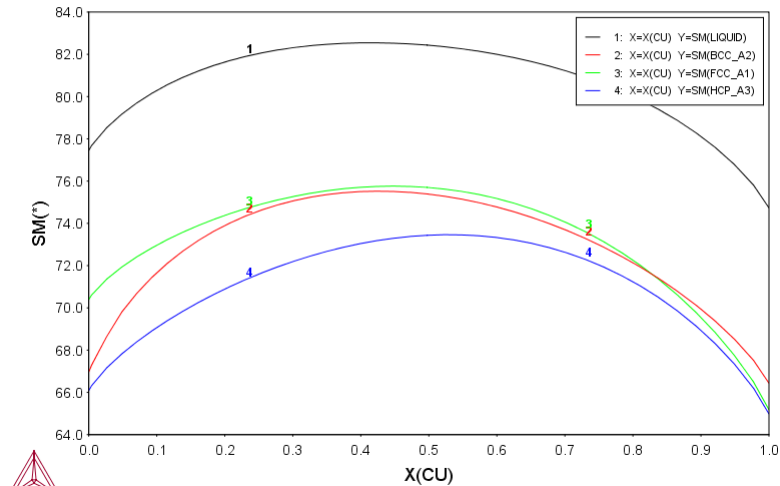


POST:  
POST:Hit RETURN to continue  
POST: @@ and finally the entropy  
POST: s-d-a y sm(\*)  
... the command in full is SET\_DIAGRAM\_AXIS  
COLUMN NUMBER /\*/: \*  
POST: set-title example 2h  
POST:  
POST: plot  
... the command in full is PLOT DIAGRAM



# example 2h

2016.05.16.13.00.47  
SSOL5: CU, FE  
T=1000, P=1E5, N=1



POST:  
POST:Hit RETURN to continue  
POST: @@ The third case: ternary system, Fe-V-C  
POST: @@ Calculate and plot Gm from the iron corner to VC  
POST: ba

... the command in full is BACK  
POLY\_3: go da  
... the command in full is GOTO\_MODULE

TDB\_SSOL5: rej sys  
... the command in full is REJECT

VA DEFINED  
GAS:G REJECTED  
REINITIATING GES5 .....

TDB\_SSOL5: d-sys fe v c  
... the command in full is DEFINE\_SYSTEM

FE V C  
DEFINED

TDB\_SSOL5: rej ph / all

... the command in full is REJECT

LIQUID:L	FCC_A1	FCC_L12
FCC_DIS	FCC_ORD	BCC_A2
BCC_B2	HCP_A3	HCP_DIS
HCP_ORD	DIAMOND_A4	TETRAGONAL_U
CBCC_A12	CUB_A13	ORTHORHOMBIC_A20
SIGMA	GRAPHITE	LAVES_C14
LAVES_C15	LAVES_C36	CEMENTITE
KSI_CARBIIDE	M23C6	M7C3
M3C2	V3C2	M5C2
MC_ETA	M4N	FECN_CHI
ALM_D019	AL5FE4	ALTA_SIGMA
ALTI	FEFD	FEFD3
FESB	FEU6	FE2U
FEZN_GAMMA_D82	FEZN4	FEZN_DELTA
FEZN_ZETA	FEUZR_DELTA	FEZR2
FEZR3	V3SI REJECTED	

TDB\_SSOL5: rest ph fcc\_a1 bcc\_a2 hcp\_a3 liq

... the command in full is RESTORE

FCC\_A1 BCC\_A2 HCP\_A3

LIQUID:L RESTORED

TDB\_SSOL5: get

... the command in full is GET\_DATA

REINITIATING GES5 .....

ELEMENTS .....

SPECIES .....

PHASES .....

... the command in full is AMEND\_PHASE\_DESCRIPTION

... the command in full is AMEND\_PHASE\_DESCRIPTION

... the command in full is AMEND\_PHASE\_DESCRIPTION

... the command in full is AMEND\_PHASE\_DESCRIPTION

PARAMETERS ...

FUNCTIONS ...

List of references for assessed data

'Data for the C-Fe system are taken from the assessment of P Gustafson, Report TRITA-MAC-0237, October 1984, Scand. J. Metall., 1985, 14, 259-267. Data for other phases not stable in the binary system are from: WM Huang: Report TRITA-MAC 411 (Rev 1989); Metall. Trans. A, 1990, 21A, 2115-2123. WM Huang: Report TRITA-MAC 441 (1990), Metall. Trans. A, 1991, 22A(9), 1911-1920. BJ Lee (1991), unpublished revision of data for C-Cr-Fe-Ni H Du and M Hillert: Z. Metallkde, 1991, 82(4), 310-316. H Du: J. Phase Equil., 1993, 14(6), 682-693. Note: Data for the V3C2 phase were modified to be 10 J/mol more positive than those for the M3C2 phase. The data for the liquid data were modified by Tatjana Buhler to prevent bcc phase from becoming stable at high temperatures. >> C-Fe '

'Data for the C-Fe-V system are taken the assessments of WM Huang: Report TRITA-MAC 432 (1990), Z. Metallkde, 1991, 82(5), 391-401. "A thermodynamic evaluation of the Fe-V-C system". BJ Lee and DN Lee: Report TRITA-MAC 474 (1991), Calphad, 1991, 15(3), 293-306. "A thermodynamic study on the Fe-V-C system". >> C-Fe-V '

'Data for the C-V system are taken from the assessment of WM Huang: Z. Metallkde, 1991, 82, (3), 174-181. "An Assessment of the V-C System". Additional data are from further work by WM Huang: Report TRITA-MAC 441 (1990), BJ Lee: Report TRITA-MAC 475 (1991). >> C-V '

'Data for the Fe-V system are from the assessments of WM Huang: TRITA-MAC 432 (Rev 1989, 1990), Z. Metallkde, 1991, 82(5), 391-401. "A thermodynamic evaluation of the Fe-V-C system", WM Huang: Met. Trans. A, 1991, 22(9), 1911-1920. "Thermodynamic properties of the Fe-Mn-V-C system". >> Fe-V '

-OK-

TDB\_SSOL5: go p-3

```

... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3: @@ set conditions for a single equilibrium
POLY_3: s-c t=1000,p=1e5,n=1,w(v)=.0015,x(c)=.001
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      7434 grid points in          0 s
Found the set of lowest grid points in        0 s
Calculated POLY solution      0 s, total time    0 s
POLY_3: l-e,,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium =      1, label A0 , database: SSOL5

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

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

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

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

FCC_A1                      Status ENTERED      Driving force 0.0000E+00
Moles 1.8638E-03, Mass 6.0520E-02, Volume fraction 0.0000E+00 Mass fractions:
V 8.23694E-01 C 1.75507E-01 FE 7.99487E-04
POLY_3:Hit RETURN to continue
POLY_3: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE      STATUS      DRIVING FORCE      MOLES
FCC_A1      ENTERED      0.000000E+00      1.863776E-03
BCC_A2      ENTERED      0.000000E+00      9.981362E-01
HCP_A3      ENTERED      -2.875358E-01      0.000000E+00
HCP_A3#2    ENTERED      -2.875358E-01      0.000000E+00
LIQUID      ENTERED      -6.510578E-01      0.000000E+00
POLY_3:Hit RETURN to continue
POLY_3: @@ Note we have several composition sets because fcc
POLY_3: @@ (and possibly hcp) can exist both as metallic and
POLY_3: @@ as carbide. However, in this case it is unnecessary
POLY_3: @@ as we are only interested in the value of the
POLY_3: @@ thermodynamic functions, not the equilibrium, and therefore
POLY_3: @@ we suspend them
POLY_3:
POLY_3: c-s p hcp_a3#2
... the command in full is CHANGE_STATUS
Status: /ENTERED/: sus
POLY_3: l-c
... the command in full is LIST_CONDITIONS
T=1000, P=1E5, N=1, W(V)=1.5E-3, X(C)=1E-3
DEGREES OF FREEDOM 0
POLY_3: @@ We would like to calculate the Gibbs energy from
POLY_3: @@ pure Fe to the corner VC. Select a line with equal
POLY_3: @@ fraction of V and C
POLY_3: s-c x(v)-x(c)=0
... the command in full is SET_CONDITION
POLY_3: s-c w(v)=none
... the command in full is SET_CONDITION
POLY_3: l-c
... the command in full is LIST_CONDITIONS
T=1000, P=1E5, N=1, X(C)=1E-3, X(V)-X(C)=0
DEGREES OF FREEDOM 0
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated      7434 grid points in          0 s
10 ITS, CPU TIME USED 0 SECONDS
POLY_3: l-e,,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium =      1, label A0 , database: SSOL5

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

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

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

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

FCC_A1                      Status ENTERED      Driving force 0.0000E+00
Moles 1.4208E-03, Mass 4.5810E-02, Volume fraction 0.0000E+00 Mass fractions:
V 8.19759E-01 C 1.78955E-01 FE 1.28625E-03
POLY_3:Hit RETURN to continue
POLY_3: @@ Set the fraction of C as axis
POLY_3: @@ The fraction of V will be the same
POLY_3: s-a-v
... the command in full is SET_AXIS_VARIABLE
Axis number: /1/: 1
Condition /NONE/: x(c)
Min value /0/: 0
Max value /1/: .5
Increment /.0125/: .0125
POLY_3: save tcex02c y
... the command in full is SAVE_WORKSPACES

```

POLY\_3: post

**POST:** @@ plot the Gm versus carbon content

**POST:** 1-p-s

## AUTOMATIC SCALING

AUTOMATIC AXIS TEXT

AXIS VARIABLES

```
POST: s-d-a x x(c)
... the command in full is SET_DIAGRAM_AXIS
```

**POST:** s-d-a y gm(\*)

... the command in full is SET\_DIAGRAM\_AXIS

COLUMN NUMBER /\*/: \*

```
POST:
POST: set-lab d
```

... the command in full is SET\_LABEL\_CURVE\_OPTION

```
POST: set-title example 2i
```

```
POST:
POST: plot
```

... the command in full is PLOT DIAGRAM

example 2i

```
2016.05.16.13.00.51
SSOL5: C, FE, V
T=1000, P=1E5, N=1, X(V)-X(C)=0
```



```
POST:
POST:Hit RETURN to continue
POST: @@ The fourth case: more partial derivatives
POST: back
```

POLY\_3: go da

... the command in full is GOTO\_MODULE

```
... the command in full is SOLID_M
TDB_SSOL5: rej sys
... the command in full is REJECT
```

VA DEFINED  
GAS:G REJECTED  
REJECTING STATE

```
REINITIATING GES5 .....
TDB_SSOL5: def-sys al cu
           the command in full is DEFINE SYSTEM
```

```
... the command in full is DEFINE_S
AL                                CU  DEFINED
TDB SSOL5: get
```

```
IDB_SSOL5: get
... the command in fu
REINITIATING GES5 .....
```

ELEMENTS . . . . .  
SPECIES . . . . .

[illegible]

```

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

```

List of references for assessed data

```

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datasets are given in the paper. The adopted assessment was derived by
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phase have been modified slightly to correct the calculated invariant
temperatures. >> Cu-Y '
'M Kowalski and PJ Spencer: J. Phase Equil., 1993, 14(4), 432-438. "
Thermodynamic reevaluation of the Cu-Zn system". Some v. minor
differences in gamma_brass data wrt SOLDERS >> Cu-Zn '

```

-OK-

**TDB\_SSOL5:** go p-3

```

... the command in full is GOTO_MODULE

```

POLY version 3.32

**POLY\_3:** s-c t=1400 p=1e5 n=1 x(al)=.1

```

... the command in full is SET_CONDITION

```

**POLY\_3:** c-e

```

... the command in full is COMPUTE_EQUILIBRIUM

```

Using global minimization procedure

```

Calculated      13716 grid points in          0 s
Found the set of lowest grid points in        0 s
Calculated POLY solution      0 s, total time    0 s

```

**POLY\_3:** l-e,,,,

```

... the command in full is LIST_EQUILIBRIUM

```

Output from POLY-3, equilibrium = 1, label A0 , database: SSOL5

Conditions:

T=1400, P=1E5, N=1, X(AL)=0.1

DEGREES OF FREEDOM 0

```

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

```

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

```

LIQUID      Status ENTERED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 5.9890E+01, Volume fraction 0.0000E+00 Mass fractions:
CU 9.54947E-01 AL 4.50529E-02

```

**POLY\_3:**Hit RETURN to continue

**POLY\_3:** @@ check the activity of aluminum

**POLY\_3:** show acr(al)

```

... the command in full is SHOW_VALUE

```

ACR(AL)=1.359263E-6

**POLY\_3:** @@ This activity value is referred to fcc Al at 298.15 K.

**POLY\_3:** @@ Set proper reference state for activities

**POLY\_3:** set-ref-state al

```

... the command in full is SET_REFERENCE_STATE

```

**Reference phase:** liq

**Temperature \*/:**

**Pressure /1E5/:**

**POLY\_3:**

**POLY\_3:** set-ref-state cu

```

... the command in full is SET_REFERENCE_STATE

```

**Reference phase:** liq

**Temperature \*/:**

**Pressure /1E5/:**

**POLY\_3:**

**POLY\_3:** show acr(al)

```

... the command in full is SHOW_VALUE

```

ACR(AL)=8.0990275E-4

**POLY\_3:** @@ This value is better. The corresponding chemical potential is

**POLY\_3:** show mur(al)

```

... the command in full is SHOW_VALUE

```

MUR(AL)=-82862.697

**POLY\_3:** @@ The relation is simply that  $\text{acr}(\text{al}) = \exp(\text{mur}(\text{al})/\text{RT})$ . Check that

**POLY\_3:** enter fun test

```

... the command in full is ENTER_SYMBOL

```

**Function:**  $\exp(\text{mur}(\text{al})/8.31451/\text{T})$ ;

**POLY\_3:** show test

```

... the command in full is SHOW_VALUE

```

TEST=8.0990275E-4

**POLY\_3:**Hit RETURN to continue

**POLY\_3:** @@ POLY allows calculation of partial derivatives of thermodynamic

**POLY\_3:** @@ quantities of original reference state with respect to fractions

**POLY\_3:** @@ that are conditions. For example

**POLY\_3:** show gm.x(al)

```

... the command in full is SHOW_VALUE

```

GM.X(AL)=-79930.097

**POLY\_3:** @@ This is not the same as the chemical potential. It actually

**POLY\_3:** @@ equals to the so-called diffusion potential:  $\mu(\text{al}) - \mu(\text{cu})$ .

**POLY\_3:** ent fun diffmu= $\mu(\text{al}) - \mu(\text{cu})$ ;

```

... the command in full is ENTER_SYMBOL

```

**POLY\_3:** show diffmu

```

... the command in full is SHOW_VALUE

```

DIFFMU=-79930.097

**POLY\_3:** @@ The relation between the chemical potential and the partial derivative is

**POLY\_3:** @@

```

POLY_3: @@ mu(al) = gm + gm.x(al) - x(al)*gm.x(al)
POLY_3: @@
POLY_3: @@ We can enter this as a function also.
POLY_3: enter fun dgdx=gm+gm.x(al)-x(al)*gm.x(al);
... the command in full is ENTER_SYMBOL
POLY_3: sh dgdx
... the command in full is SHOW_VALUE

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

DGDx=-157243.97
POLY_3: sh mu(al)
... the command in full is SHOW_VALUE
MU(AL)=-157243.97
POLY_3: @@ Partial entropy is the negative of mu(al).t
POLY_3: ent fun ps=-mu(al).t;
... the command in full is ENTER_SYMBOL
POLY_3: sh ps
... the command in full is SHOW_VALUE

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

PS=95.218667
POLY_3: @@ Partial enthalpy is h = g + s*t
POLY_3: enter fun ph=mu(al)+ps*t;
... the command in full is ENTER_SYMBOL
POLY_3: sh ph
... the command in full is SHOW_VALUE

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

PH=-23937.838
POLY_3: @@ Partial enthalpy can also be calculated in a similar way as chemical
POLY_3: @@ potential
POLY_3: @@ partial enthalpy = hm + hm.x(al) - x(al)*hm.x(al)
POLY_3: ent fun ph1=hm+hm.x(al)-x(al)*hm.x(al);
... the command in full is ENTER_SYMBOL
POLY_3: sh ph1
... the command in full is SHOW_VALUE

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

PH1=-23937.838
POLY_3: @@ As can be seen, ph1 = ph.
POLY_3: @@ Another useful quantity is mu(al).x(al). That is related to
POLY_3: @@ the thermodynamic factor and part of the diffusion coefficient.
POLY_3: show mu(al).x(al)
... the command in full is SHOW_VALUE
MU(AL).X(AL)=324789.82
POLY_3:
POLY_3: set-inter
... the command in full is SET_INTERACTIVE
POLY_3:

```

tcex03

```
AboutMACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex03\tcex03.TCM" set-echo
SYS: @@
SYS: @@
SYS: @@ Calculation of an isothermal section using TERNARY module
SYS: @@
SYS: set-log ex03,,
SYS:
SYS: go tern
... the command in full is GOTO_MODULE

Quick ternary phase diagram calculation module

THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
L12_FCC B2_BCC B2_VACANCY
HIGH_SIGMA DICTRA_FCC_A1 REJECTED
Current database: Iron Demo Database

VA /- DEFINED
Database: /FEDEMO/: FEDEMO
First element: ?
The following assessed systems
C-CR-FE C-CR C-FE CR-FE

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

List of references for assessed data

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Sigma model'
-OK-
The condition X(CR)=.1234 created
The condition X(FE)=.1234 created
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
```

Working hard

Generating start point	11		
Generating start point	12		
Generating start point	13		
Generating start point	14		
Generating start point	15		
Generating start point	16		
Generating start point	17		
Generating start point	18		
Generating start point	19		
Generating start point	20		
Generating start point	21		

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

Phase region boundary	2 at:	2.749E-01	7.508E-02
** GRAPHITE			
** M3C2			
M7C3			

Phase region boundary	3 at:	5.749E-01	7.508E-02
** M3C2			
M7C3			
Calculated		18	equilibria

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

Phase region boundary	5 at:	2.749E-01	7.508E-02
** GRAPHITE			
M7C3			
Calculated.		20	equilibria

Phase region boundary	6 at:	9.248E-02	2.575E-01
** CEMENTITE			
** GRAPHITE			
M7C3			

Phase region boundary	7 at:	1.406E-01	5.844E-01
** CEMENTITE			
M7C3			
Calculated.		5	equilibria

Phase region boundary	8 at:	1.754E-01	5.496E-01
** LIQUID			
** CEMENTITE			
M7C3			

Phase region boundary	9 at:	1.452E-01	6.174E-01
** LIQUID			
M7C3			
Calculated.		3	equilibria

Phase region boundary	10 at:	1.571E-01	6.091E-01
** LIQUID			
** FCC_A1#2			
M7C3			

Phase region boundary	11 at:	1.436E-01	6.656E-01
** FCC_A1			
M7C3			
Calculated.		32	equilibria

Phase region boundary	12 at:	3.786E-01	4.505E-01
** BCC_A2			
** FCC_A1			
M7C3			

Phase region boundary	13 at:	3.849E-01	4.619E-01
** BCC_A2			
M7C3			
Calculated.		5	equilibria

Phase region boundary	14 at:	4.217E-01	4.253E-01
** BCC_A2			
** M23C6			
M7C3			

Phase region boundary	15 at:	5.511E-01	1.954E-01
** M23C6			
M7C3			
Calculated		30	equilibria

Phase region boundary	16 at:	4.085E-01	4.850E-01
BCC_A2			
** M23C6			
Calculated		56	equilibria

Phase region boundary	17 at:	2.122E-01	7.714E-01
** BCC_A2			
FCC_A1			
Calculated		24	equilibria

Phase region boundary	18 at:	5.747E-02	8.179E-01
LIQUID			
** FCC_A1			
Calculated		24	equilibria

Phase region boundary	19 at:	9.527E-02	6.924E-01
** LIQUID			
CEMENTITE			
Calculated.		9	equilibria

Phase region boundary	20 at:	4.556E-02	7.341E-01
** LIQUID			
CEMENTITE			
** GRAPHITE			

Phase region boundary	21 at:	2.996E-02	3.450E-01
CEMENTITE			
** GRAPHITE			
Calculated.		3	equilibria

Terminating at known equilibrium

Phase region boundary 22 at: 1.560E-02 3.890E-01  
LIQUID  
\*\* GRAPHITE  
Calculated 23 equilibria

Phase region boundary 23 at: 1.750E-01 1.750E-01  
\*\* GRAPHITE  
M7C3  
Calculated. 10 equilibria  
Terminating at known equilibrium

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

Phase region boundary 25 at: 1.750E-01 1.750E-01  
\*\* GRAPHITE  
M7C3  
Calculated. 10 equilibria  
Terminating at known equilibrium

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

Phase region boundary 27 at: 2.749E-01 7.508E-02  
\*\* GRAPHITE  
M7C3  
Calculated. 20 equilibria  
Terminating at known equilibrium

Phase region boundary 28 at: 5.749E-01 7.508E-02  
\*\* M3C2  
M7C3  
Calculated 21 equilibria

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

Phase region boundary 30 at: 6.432E-01 6.818E-03  
\*\* M3C2  
M7C3  
Calculated. 8 equilibria  
Terminating at known equilibrium

Phase region boundary 31 at: 8.931E-01 3.310E-03  
BCC\_A2  
\*\* M23C6  
Calculated 11 equilibria

Phase region boundary 32 at: 8.931E-01 3.310E-03  
BCC\_A2  
\*\* M23C6  
Calculated. 50 equilibria  
Terminating at known equilibrium

Phase region boundary 33 at: 1.172E-02 3.945E-01  
LIQUID  
\*\* GRAPHITE  
Calculated. 2 equilibria  
Terminating at known equilibrium

Phase region boundary 34 at: 1.172E-02 3.945E-01  
LIQUID  
\*\* GRAPHITE  
Calculated 24 equilibria

Phase region boundary 35 at: 6.066E-03 4.024E-01  
LIQUID  
\*\* GRAPHITE  
Calculated. 3 equilibria  
Terminating at known equilibrium

Phase region boundary 36 at: 6.066E-03 4.024E-01  
LIQUID  
\*\* GRAPHITE  
Calculated 19 equilibria

Phase region boundary 37 at: 1.253E-02 8.670E-01  
\*\* LIQUID  
FCC\_A1  
Calculated 12 equilibria

Phase region boundary 38 at: 1.253E-02 8.670E-01  
\*\* LIQUID  
FCC\_A1  
Calculated. 7 equilibria  
Terminating at known equilibrium

Phase region boundary 39 at: 4.511E-01 4.428E-01  
BCC\_A2  
\*\* M23C6  
Calculated 57 equilibria

Phase region boundary 40 at: 4.511E-01 4.428E-01  
BCC\_A2  
\*\* M23C6  
Calculated. 6 equilibria  
Terminating at known equilibrium

Phase region boundary 41 at: 6.796E-01 2.160E-01  
BCC\_A2  
\*\* M23C6  
Calculated 35 equilibria

Phase region boundary 42 at: 6.796E-01 2.160E-01  
BCC\_A2  
\*\* M23C6  
Calculated. 28 equilibria  
Terminating at known equilibrium



```

*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex03\ISOT
HER.POLY3
CPU time for mapping          3 seconds

```

POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POSTPROCESSOR VERSION 3.2

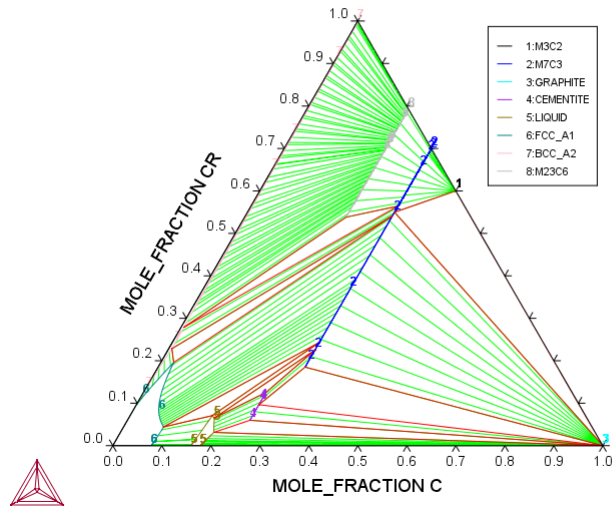
Setting automatic diagram axes

FE-C-CR at T=1473.15 K

```

2016.05.16.13.03.01
FEDEMO: C, CR, FE
T=1473.15, P=1E5, N=1

```



```

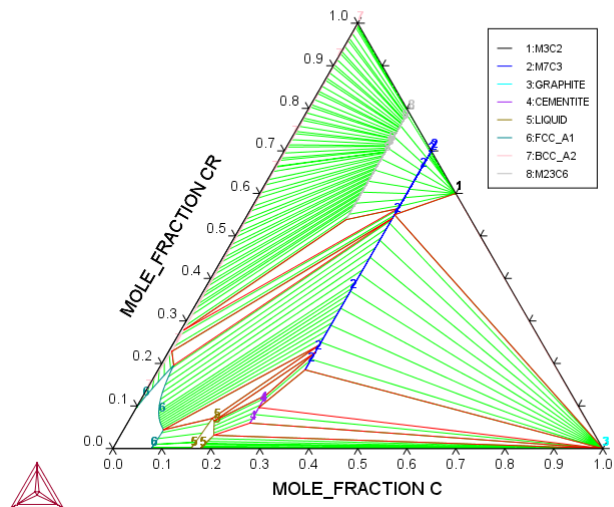
POST:
POST: set-title example 3a
POST: plot
... the command in full is PLOT DIAGRAM
example 3a

```

```

2016.05.16.13.03.02
FEDEMO: C, CR, FE
T=1473.15, P=1E5, N=1

```



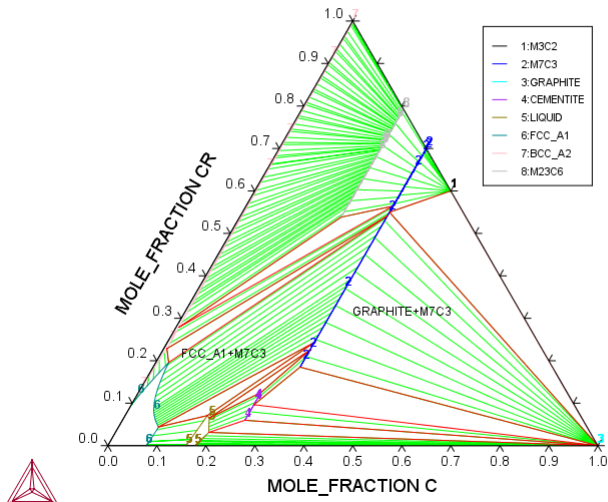
```

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

```

2016.05.16.13.03.02  
 FEDEMO: C, CR, FE  
 T=1473.15, P=1E5, N=1

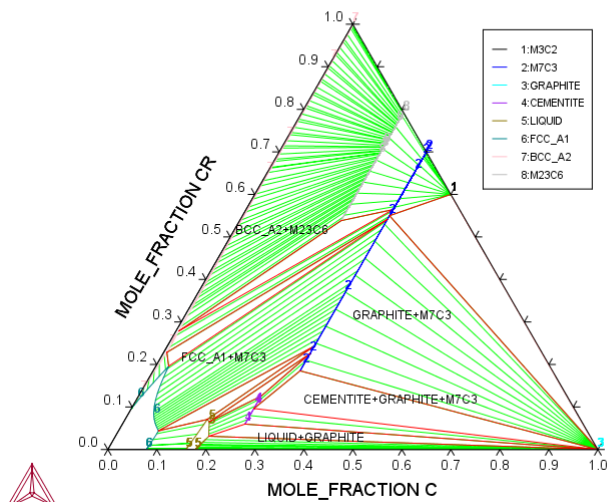
example 3b



```
POST:
POST:Hit RETURN to continue
POST: add .3 .01
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Using already calculated grid
Found the set of lowest grid points in      0 s
Calculated POLY solution      0 s, total time  0 s
Stable phases are: LIQUID+GRAPHITE
Text size: /.36/:
POST: add .35 .1
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Using already calculated grid
Found the set of lowest grid points in      0 s
Calculated POLY solution      1 s, total time  1 s
Stable phases are: CEMENTITE+GRAPHITE+M7C3
Text size: /.36/:
POST: add .01 .5
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Using already calculated grid
Found the set of lowest grid points in      0 s
Calculated POLY solution      0 s, total time  0 s
Stable phases are: BCC_A2+M23C6
Text size: /.36/:
POST: set-title example 3c
POST:
POST: plot
... the command in full is PLOT DIAGRAM
```

example 3c

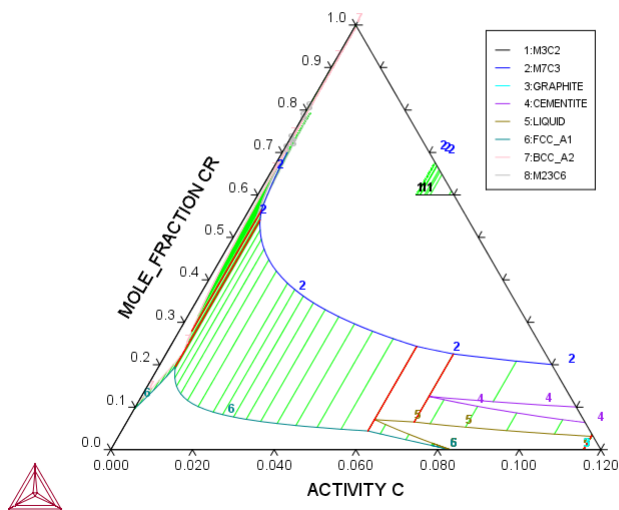
2016.05.16.13.03.03  
 FEDEMO: C, CR, FE  
 T=1473.15, P=1E5, N=1



```
POST:
POST:Hit RETURN to continue
POST: @@ We can try the same exercise as in example 1, use
POST: @@ carbon activity as one axis
POST: s-d-a x ac c
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 3d
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
```

2016.05.16.13.03.04  
 FEDEMO: C, CR, FE  
 T=1473.15, P=1E5, N=1

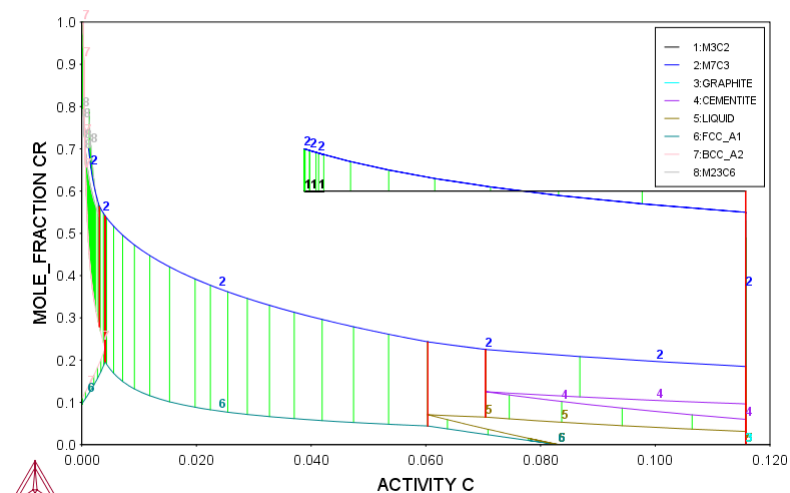
example 3d



POST:  
 POST:Hit RETURN to continue  
 POST: @@ With these axes it is better to have a square diagram!  
 POST: s-dia-type  
 ... the command in full is SET\_DIAGRAM\_TYPE  
 TRIANGULAR DIAGRAM (Y OR N) /N/: N  
 CREATE TETRAHEDRON WRML FILE (Y OR N) /N/:  
 POST:  
 POST: set-title example 3e  
 POST:  
 POST: plot  
 ... the command in full is PLOT DIAGRAM

example 3e

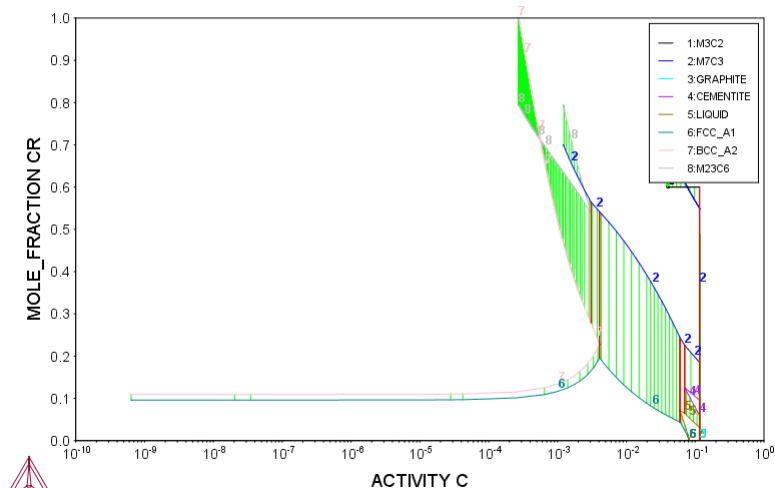
2016.05.16.13.03.04  
 FEDEMO: C, CR, FE  
 T=1473.15, P=1E5, N=1



POST:  
 POST:Hit RETURN to continue  
 POST: @@ The activity axis is probably better as logarithmic  
 POST: s-a-ty x  
 ... the command in full is SET\_AXIS\_TYPE  
 AXIS TYPE /LINEAR/: log  
 POST: set-title example 3f  
 POST:  
 POST: plot  
 ... the command in full is PLOT\_DIAGRAM

# example 3f

2016.05.16.13.03.04  
FEDEMO: C, CR, FE  
T=1473.15, P=1E5, N=1



POST:  
POST:Hit RETURN to continue  
POST: @@ In order for pure graphite to have activity one, the reference  
POST: @@ state of C should be set to graphite. In addition,  
POST: @@ the solubility lines now cross! Is the diagram wrong?  
POST: @@ No, in this case one should not use the mole fraction of Cr  
POST: @@ but the metallic fraction. This can be set by setting  
POST: @@ the status of C to "special". All species set as special  
POST: @@ will be excluded from the summation of fractions.  
POST: @@ The special status is set in the POLY module  
POST: ba

... the command in full is BACK  
SYS: go p-3  
... the command in full is GOTO\_MODULE

POLY\_3:  
POLY\_3: s-r-s  
... the command in full is SET\_REFERENCE\_STATE

Component: c  
Reference phase: gra  
Temperature /\*/  
Pressure /1E5/  
POLY\_3: ch-st

... the command in full is CHANGE STATUS  
For phases, species or components? /PHASES/: c  
Name(s): c  
Status: /ENTERED/: ?

Status

The new status to be assigned must be given.

- \* For species, the values ENTERED or SUSPENDED can be used.
- \* For components, the status ENTERED, SUSPENDED or SPECIAL can be given.  
SPECIAL means that this component will be excluded from sums for mole fractions and mass fractions.
- \* For phases, the status ENTERED, SUSPENDED, DORMANT or FIXED can be given.  
DORMANT means the same as suspended but the driving force will be calculated. FIXED means that it is a condition that the phase is stable at a certain amount.

Note that only component(s) may have the status SPECIAL, which implies that they will not be included in summations for mole or mass fractions. For instance, for the so-called "u" fractions or other normalized fractions, when one or more of the components are excluded from the summation, one must specify which component(s) should be excluded from the calculation of mole or mass fraction. This component status is particularly useful when calculating paraequilibrium states. Such component(s) are normally interstitial component, and must have the status SPECIAL. This is assigned by the CHANGE\_STATUS command. For example, to obtain the metallic fraction in a system with as an interstitial component, one can set the component status for carbon as SPECIAL:  
Change\_status comp C=special

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

- \* The phase amount variables, NP(phase), BP(phase) and VP(phase), as well as all their M/W/V-suffixed quantities, should not be used as conditions. Instead, one can use the CHANGE\_STATUS command to set a relevant condition, e.g., CHANGE\_STATUS phase <phase>=fix <amount> where the fixed <amount> is roughly the same as the F-suffixed quantity "NPF(phase)".
- \* The "NPF(phase)" quantity is the normalized mole number of components (per mole formula unit) of the specific phase in the defined system, which unlike other F-suffixed state variables [e.g., GF(phase), HF(phase) and DGF(phase)] can not be directly applied in any POLY command, implying that it can not be directly evaluated or listed/shown. If intended to shown such a normalized phase amount value in an equilibrium state, one should instead use a properly-entered symbol (function or variable), for instance,  
NPFabc = NP(abc)/NA  
or NPFabc = NPM(abc)/NA\*N  
N is the total system size (in mole). The NA value is a quantity that is phase-dependent (and sometimes also equilibrium-dependent for ionic solution phases), and is the total atomic number in a mole-formula-unit of the specific phase abc (excluding interstitial component and, of course, vacancy).

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

```
LIQUID (C,Cr,CrO3/2,Fe,FeO,FeO3/2,N,Ni,NiO)1 --> NA = 1
FCC_A1 (Cr,Fe,Ni)1(Va,C,N,O)1 --> NA = 1
BCC_A2 (Cr,Fe,Ni)1(Va,C,N,O)3 --> NA = 1
SIGMA (Fe,Ni)8(Cr)4(Cr,Fe,Ni)18 --> NA = 30
```

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

```
IONIC LIQ (Cr+3,Fe+2,Ni+2)p(Va,C,N,O-2,FeO3/2)q
```

the evaluation of its NA value becomes even more complicated,  
 $NA = p \cdot q \cdot y(C\_2ndSite) + q \cdot (N\_2ndSite) + q \cdot (O-2\_2ndSite) + q \cdot (FeO3/2\_2ndSite)$   
 where the stoichiometric coefficients p and q are also dependent upon the real equilibrium state (rather than having fixed values in the system). Similar situations occur for other (solid) phases which are described by multiple-sublattice model with ionic constituents, such as SPINEL and HALITE phases in some databases.

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

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

Therefore, a FIXED-status for a liquid phase being unity does not necessarily imply that it is a liquidus equilibrium state (where the liquid phase is in equilibrium with some solid phases but the liquid phase takes all the mass in the defined system). A unity value for setting the liquid phase status in calculating liquidus equilibrium state can only be used when the liquid mixture phase has been predefined as a single-sublattice solution phase (such as metallic liquid phase in multicomponent alloy systems) and the total system size as one mole (i.e., N=1).

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

Status: /ENTERED/: special

POLY\_3:

POLY\_3: post

POST:

POST: set-title example 3g

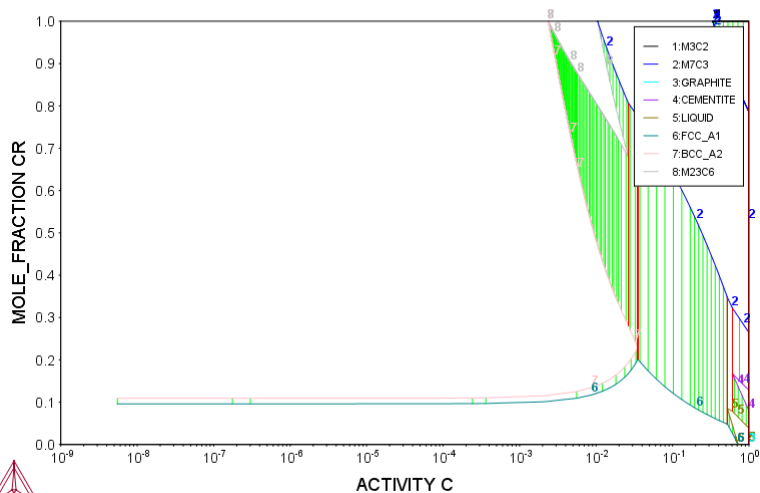
POST:

POST: plot

... the command in full is PLOT DIAGRAM

example 3g

2016.05.16.13.03.05  
 FEDEMO: C, CR, FE  
 T=1473.15, P=1E5, N=1



POST:  
 POST:Hit RETURN to continue

POST: @@ Finally scale

POST: s-s x n .001 1

... the command in full is SET\_SCALING\_STATUS

POST: set-title example 3h

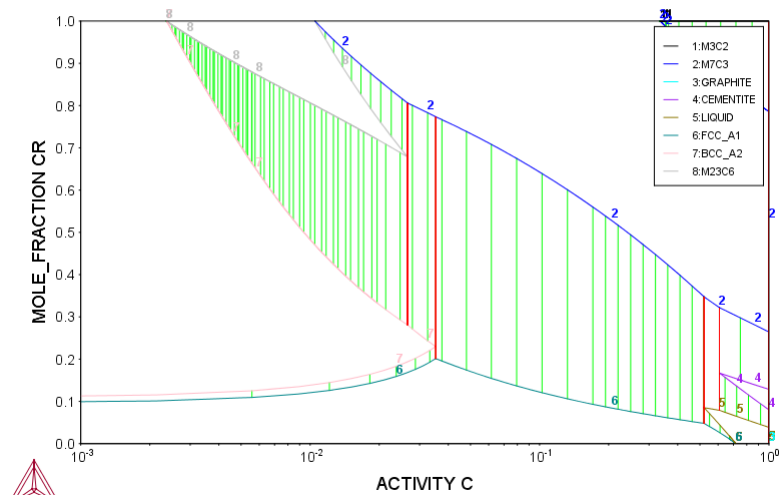
POST:

POST: plot

... the command in full is PLOT DIAGRAM

### example 3h

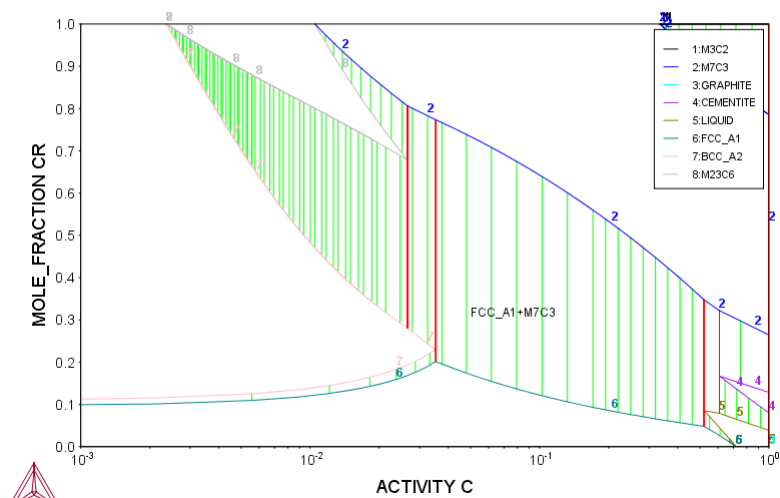
2016.05.16.13.03.05  
FEDEMO: C, CR, FE  
T=1473.15, P=1E5, N=1



```
POST:
POST:Hit RETURN to continue
POST: @@ This kind of diagram is useful to understand diffusion paths.
POST: @@
POST: @@ The phase labels were lost when we changed axis
POST: @@ One may add them again
POST: add .05 .3
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Testing POLY result by global minimization procedure
Calculated      16532 grid points in      0 s
Stable phases are: FCC_A1+M7C3
Text size: /.36/:
POST: set-title example 3i
POST:
POST: plot
... the command in full is PLOT DIAGRAM
```

### example 3i

2016.05.16.13.03.06  
FEDEMO: C, CR, FE  
T=1473.15, P=1E5, N=1



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

tcex04

About License library version: 8.5.1.0017  
Linked: Mon May 16 09:31:44 2016

```
SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex04\tcex04.TCM"SYS: set-echo
SYS: @@
SYS: @@
SYS: @@ Calculation of the miscibility gap in Fe-Cr
SYS: @@
SYS: set-log ex04,,,
SYS:
SYS: go data
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
LI2 FCC B2_BCC B2_VACANCY
HIGH_SIGMA DICTRA_FCC_A1 REJECTED
TDB_TCFE8: sw FEDEMO
... the command in full is SWITCH_DATABASE
Current database: Iron Demo Database

VA /- DEFINED
TDB_FEDEMO: def-sys
... the command in full is DEFINE_SYSTEM
ELEMENTS: fe cr CR DEFINED
TDB_FEDEMO: l-sys
... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:
LIQUID:L :CR FE:
BCC_A2 :CR FE:VA:
CHI_A12 :CR FE:CR:CR FE:
FCC_A1 :CR FE:VA:
HCP_A3 :CR FE:VA:
LAVES_PHASE_C14 :CR FE:CR FE:
SIGMA :CR FE:CR:CR FE:
TDB_FEDEMO: rej ph /all
... the command in full is REJECT
LIQUID:L BCC_A2 CHI_A12
FCC_A1 HCP_A3 LAVES_PHASE_C14
SIGMA REJECTED
TDB_FEDEMO: rest ph liquid fcc_a1 bcc_a2 sigma
... the command in full is RESTORE
LIQUID:L FCC_A1 BCC_A2
SIGMA RESTORED
TDB_FEDEMO: get
... the command in full is GET_DATA
REINITIATING GES5 .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
Molar volumes'
'X.-G. Lu et al. Calphad 29 (2005) 49-55, Fe P-T diagram'
'B.-J. Lee, Calphad (1993); revision of Fe-Cr and Fe-Ni liquid'
'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
'J.-O. Andersson and B. Sundman, Calphad, 11 (1987), 83-92; TRITA 0270
(1986); CR-FE'
'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
Sigma model'

-OK-
TDB_FEDEMO: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3: l-st
... the command in full is LIST_STATUS
Option /CPS/:
*** STATUS FOR ALL COMPONENTS
COMPONENT STATUS REF. STATE T(K) P(Pa)
VA ENTERED SER
CR ENTERED SER
FE ENTERED SER
*** STATUS FOR ALL PHASES
PHASE STATUS DRIVING FORCE MOLES
SIGMA ENTERED 0.000000E+00 0.000000E+00
FCC_A1 ENTERED 0.000000E+00 0.000000E+00
BCC_A2 ENTERED 0.000000E+00 0.000000E+00
LIQUID ENTERED 0.000000E+00 0.000000E+00
*** STATUS FOR ALL SPECIES
CR ENTERED FE ENTERED VA ENTERED
POLY_3:Hit RETURN to continue
POLY_3: @@ There is a miscibility gap in BCC Fe-Cr.
POLY_3: @@ Let us first calculate the low temperature region.
POLY_3: s-c x(cr)=.6 t=700 p=101325 n=1
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 2230 grid points in 0 s
Found the set of lowest grid points in 0 s
Creating a new composition set BCC_A2#2
Calculated POLY solution 0 s, total time 0 s
POLY_3: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium = 1, label A0 , database: FEDEMO

Conditions:
```

```

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

Temperature 700.00 K ( 426.85 C), Pressure 1.013250E+05
Number of moles of components 1.00000E+00, Mass in grams 5.35364E+01
Total Gibbs energy -2.30658E+04, Enthalpy 1.31794E+04, Volume 7.26641E-06

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

BCC_A2#2              Status ENTERED      Driving force 0.0000E+00
Moles 6.0112E-01, Mass 3.1435E+01, Volume fraction 6.0312E-01 Mass fractions:
CR 9.17570E-01 FE 8.24301E-02

BCC_A2              Status ENTERED      Driving force 0.0000E+00
Moles 3.9888E-01, Mass 2.2102E+01, Volume fraction 3.9688E-01 Mass fractions:
FE 8.93484E-01 CR 1.06516E-01
POLY 3:Hit RETURN to continue
POLY 3: @@ Now make a calculation at a higher temperature
POLY 3: s-c t=900
... the command in full is SET_CONDITION
POLY 3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 2230 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY 3: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium = 1, label A0 , database: FEDEMO

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

Temperature 900.00 K ( 626.85 C), Pressure 1.013250E+05
Number of moles of components 1.00000E+00, Mass in grams 5.35364E+01
Total Gibbs energy -3.49346E+04, Enthalpy 2.36848E+04, Volume 7.26400E-06

Component      Moles      W-Fraction  Activity   Potential  Ref.stat
CR              6.0000E-01  5.8274E-01 1.2779E-02 -3.2626E+04 SER
FE              4.0000E-01  4.1726E-01 5.9088E-03 -3.8398E+04 SER

SIGMA              Status ENTERED      Driving force 0.0000E+00
Moles 6.4245E-01, Mass 3.4609E+01, Volume fraction 6.3947E-01 Mass fractions:
FE 5.04665E-01 CR 4.95335E-01

BCC_A2              Status ENTERED      Driving force 0.0000E+00
Moles 3.5755E-01, Mass 1.8927E+01, Volume fraction 3.6053E-01 Mass fractions:
CR 7.42558E-01 FE 2.57442E-01
POLY 3:Hit RETURN to continue
POLY 3: @@ The Fe-Cr phase diagram has three non-connected two-phase regions.
POLY 3:
POLY 3: s-a-v 1 x(cr)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: 1
Increment /.025/:
POLY 3: s-a-v 2
... the command in full is SET_AXIS_VARIABLE
Condition /NONE/: t
Min value /0/: 600
Max value /1/: 2200
Increment /40/:
POLY 3: @@ Always a SAVE command before MAP (or STEP) unless
POLY 3: @@ you want to overlay this calculation with an earlier one
POLY 3: save tcex04 y
... the command in full is SAVE_WORKSPACES
POLY 3: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

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

Phase region boundary 1 at: 1.067E-02 1.169E+03

```



```

    BCC_A2
** FCC_A1
Calculated
12 equilibria

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

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

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

Phase region boundary 5 at: 5.192E-01 7.875E+02
    BCC_A2
** BCC_A2#2
** SIGMA
Phase region boundary 6 at: 6.763E-01 7.875E+02
    BCC_A2
** SIGMA
Calculated
50 equilibria

Phase region boundary 7 at: 6.763E-01 7.875E+02
    BCC_A2
** SIGMA
Calculated.
106 equilibria
Terminating at known equilibrium

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

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

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

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

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

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

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

Phase region boundary 15 at: 1.224E-02 1.663E+03
    BCC_A2
    FCC_A1
Calculated
44 equilibria

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

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

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

Phase region boundary 19 at: 3.471E-01 1.807E+03
    LIQUID
** BCC_A2
Calculated
37 equilibria

Phase region boundary 20 at: 3.471E-01 1.807E+03
    LIQUID
** BCC_A2
Calculated
62 equilibria

Phase region boundary 21 at: 6.881E-01 2.007E+03
    LIQUID
** BCC_A2
Calculated
68 equilibria

Phase region boundary 22 at: 6.881E-01 2.007E+03
    LIQUID
** BCC_A2
Calculated
37 equilibria

Phase region boundary 23 at: 9.910E-01 2.176E+03

```

```
LIQUID
** BCC_A2
Calculated          90 equilibria

Phase region boundary 24 at:  9.910E-01  2.176E+03
LIQUID
** BCC_A2
Calculated          12 equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex04\tcex
04.POLY3
CPU time for mapping          2 seconds
```

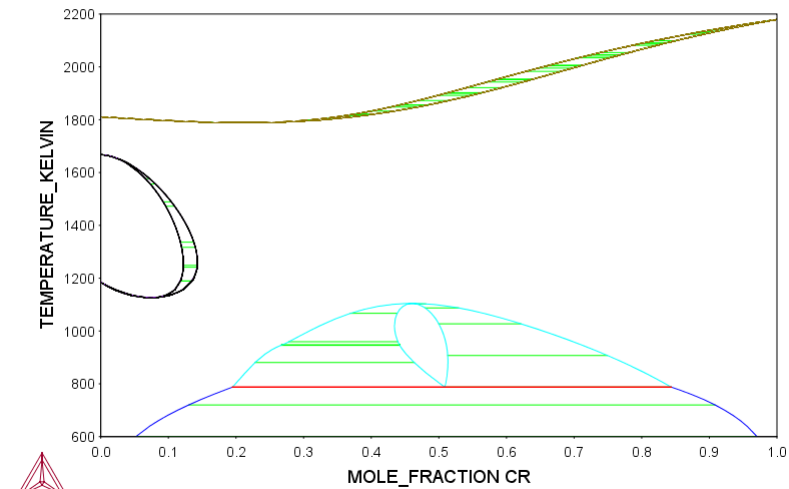
POLY\_3:  
POLY\_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST:  
POST: s-t-s 6  
... the command in full is SET\_TIELINE\_STATUS  
POST: set\_title example 4a  
POST: plot  
... the command in full is PLOT DIAGRAM  
example 4a

2016.05.16.13.05.16  
FEDEMO: CR,FE  
P=1.01325E5,N=1



POST:  
POST: set-inter  
... the command in full is SET\_INTERACTIVE\_MODE  
POST:

tcex05

#### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software (build 9533) running on WinNT 64-bit wordlength  
Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118  
License library version: 8.5.1.0017  
Linked: Mon May 16 09:31:44 2016

SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex05\tcex05.TCM"SYS: set-echo

SYS:

SYS: @@ Calculation of a vertical section

SYS: @@ in the Al-Cu-Si system

SYS: @@ Calculation of a vertical section from Al to 10% cu2Si

SYS: @@

SYS: set-log ex05,,

SYS: go da

... the command in full is GOTO\_MODULE

THERMODYNAMIC DATABASE module

Current database: Steels/Fe-Alloys v8.0

VA DEFINED

L12\_FCC

B2\_BCC

B2\_VACANCY

HIGH\_SIGMA

DICTRA\_FCC\_A1 REJECTED

TDB\_TCFE8: sw ALDEMO

... the command in full is SWITCH\_DATABASE

Current database: Aluminum Demo Database

VA /- DEFINED

TDB\_ALDEMO: def-sys al Cu si

... the command in full is DEFINE\_SYSTEM

AL CU SI

DEFINED

TDB\_ALDEMO: get

... the command in full is GET\_DATA

REINITIATING GES5 .....

ELEMENTS .....

SPECIES .....

PHASES .....

... the command in full is AMEND\_PHASE\_DESCRIPTION

... the command in full is AMEND\_PHASE\_DESCRIPTION

... the command in full is AMEND\_PHASE\_DESCRIPTION

... the command in full is AMEND\_PHASE\_DESCRIPTION

PARAMETERS ...

FUNCTIONS ....

List of references for assessed data

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'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'

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'C.-Y. He, Calphad, 33, 200-210 (2009), Al-Cu-Si'

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'Hai-Lin Chen, in TCAL2.0, Extrapolations, assumptions

adjustment'

'J.R. Zhao, Y. Du, in , 2010, Sn-Sr, Cu-Mg-Si'

'L. Kjellqvist, Thermo-Calc Software AB, 2012; Molar volumes'

'W.H. Sun, unpublished (2010), Cu-Si-Zn, Cu-Ni-Zn'

-OK-

TDB\_ALDEMO: go p-3

... the command in full is GOTO\_MODULE

POLY version 3.32

POLY\_3: s-c t=1000,p=1e5,n=1

... the command in full is SET\_CONDITION

POLY\_3: @@ We shall calculate along a line where the cu content is twice

POLY\_3: @@ that of the Si content, this can be used as a condition.

POLY\_3: @@ Note that the whole equation must be given before the equal sign.

POLY\_3: @@ It is wrong to write s-c x(cu)=2\*x(si).

POLY\_3: s-c x(cu)-2\*x(si)=0

... the command in full is SET\_CONDITION

POLY\_3: l-c

... the command in full is LIST\_CONDITIONS

T=1000, P=1E5, N=1, X(CU)-2\*X(SI)=0

DEGREES OF FREEDOM 1

POLY\_3: s-c w(si)=0.05

... the command in full is SET\_CONDITION

POLY\_3: c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Normal POLY minimization, not global

Testing POLY result by global minimization procedure

Calculated 16528 grid points in 0 s

115 ITS, CPU TIME USED 0 SECONDS

POLY\_3: l-e

... the command in full is LIST\_EQUILIBRIUM

OUTPUT TO SCREEN OR FILE /SCREEN/:

Options /VWCS/: VWCS

Output from POLY-3, equilibrium = 1, label A0 , database: ALDEMO

Conditions:

T=1000, P=1E5, N=1, X(CU)-2\*X(SI)=0, W(SI)=5E-2

DEGREES OF FREEDOM 0

Temperature 1000.00 K ( 726.85 C), Pressure 1.000000E+05

Number of moles of components 1.00000E+00, Mass in grams 3.10908E+01

Total Gibbs energy -5.01533E+04, Enthalpy 2.90243E+04, Volume 1.00919E-05

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
-----------	-------	------------	----------	-----------	----------

AL	8.3395E-01	7.2374E-01	4.7926E-03	-4.4405E+04	SER
----	------------	------------	------------	-------------	-----

CU	1.1070E-01	2.2626E-01	9.6970E-06	-9.5980E+04	SER
----	------------	------------	------------	-------------	-----

```

SI                      5.5351E-02  5.0000E-02  4.4065E-03  -4.5103E+04  SER

LIQUID                      Status ENTERED      Driving force  0.0000E+00
Moles 1.0000E+00, Mass 3.1091E+01, Volume fraction 1.0000E+00  Mass fractions:
AL  7.23737E-01  CU  2.26263E-01  SI  5.00000E-02
POLY_3:0?<Hit_return_to_continue>
POLY_3: ?
... the command in full is HELP
ADD_INITIAL_EQUILIBRIUM  EXIT              REINITIATE_MODULE
ADVANCED_OPTIONS        GOTO_MODULE        SAVE_WORKSPACES
AMEND_STORED_EQUILIBRIA HELP              SELECT_EQUILIBRIUM
BACK                    INFORMATION         SET_ALL_START_VALUES
CHANGE_STATUS           LIST_AXIS_VARIABLE SET_AXIS_VARIABLE
COMPUTE_EQUILIBRIUM    LIST_CONDITIONS  SET_CONDITION
COMPUTE_TRANSITION     LIST_EQUILIBRIUM  SET_INPUT_AMOUNTS
CREATE_NEW_EQUILIBRIUM LIST_INITIAL_EQUILIBRIA SET_INTERACTIVE
DEFINE_COMPONENTS      LIST_STATUS     SET_NUMERICAL_LIMITS
DEFINE_DIAGRAM         LIST_SYMBOLS      SET_REFERENCE_STATE
DEFINE_MATERIAL        LOAD_INITIAL_EQUILIBRIUM SET_START_CONSTITUTION
DELETE_INITIAL_EQUILIB MACRO_FILE_OPEN    SET_START_VALUE
DELETE_SYMBOL          MAP                SHOW_VALUE
ENTER_SYMBOL           POST               STEP_WITH_OPTIONS
EVALUATE_FUNCTIONS    READ_WORKSPACES    TABULATE
POLY_3: s-a-v 1
... the command in full is SET_AXIS_VARIABLE
Condition /NONE/: w(sI)
Min value /0/: 0
Max value /1/: .1
Increment /.0025/: .0025
POLY_3: s-a-v 2
... the command in full is SET_AXIS_VARIABLE
Condition /NONE/: t
Min value /0/: 500
Max value /1/: 1300
Increment /20/: 10
POLY_3: l-a-v
... the command in full is LIST_AXIS_VARIABLE
Axis No 1: W(SI)          Min: 0          Max: 0.1          Inc: 2.5E-3
Axis No 2: T              Min: 500         Max: 1300         Inc: 10
POLY_3:0?<Hit_return_to_continue>
POLY_3: save tcex05 y
... the command in full is SAVE_WORKSPACES
POLY_3: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Tie-lines not in the plane of calculation
Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16

Phase region boundary 1 at: 5.000E-02 8.204E+02
** FCC_L12
LIQUID
Calculated 37 equilibria

Phase region boundary 2 at: 5.000E-02 8.204E+02
** FCC_L12
LIQUID
Calculated. 4 equilibria

Phase region boundary 3 at: 5.713E-02 7.965E+02
** AL2CU_C16
** FCC_L12
LIQUID

Phase region boundary 4 at: 5.713E-02 7.965E+02
AL2CU_C16
** FCC_L12
LIQUID
Calculated. 2 equilibria

Phase region boundary 5 at: 5.852E-02 7.950E+02
AL2CU_C16
** DIAMOND_A4
** FCC_L12
LIQUID

Phase region boundary 6 at: 1.036E-01 7.950E+02
AL2CU_C16
DIAMOND_A4
** FCC_L12

Phase region boundary 7 at: 1.147E-02 7.950E+02
** AL2CU_C16

```

DIAMOND\_A4  
 FCC\_L12  
 Calculated.. 31 equilibria  
 Terminating at axis limit.

Phase region boundary 8 at: 1.036E-01 7.950E+02  
 AL2CU\_C16  
 DIAMOND\_A4  
 \*\* LIQUID

Phase region boundary 9 at: 5.852E-02 7.950E+02  
 AL2CU\_C16  
 \*\* DIAMOND\_A4  
 LIQUID  
 Calculated. 2 equilibria

Phase region boundary 10 at: 6.069E-02 8.026E+02  
 \*\* AL2CU\_C16  
 \*\* DIAMOND\_A4  
 LIQUID

Phase region boundary 11 at: 6.069E-02 8.026E+02  
 \*\* DIAMOND\_A4  
 LIQUID  
 Calculated.. 18 equilibria  
 Terminating at axis limit.

Phase region boundary 12 at: 6.069E-02 8.026E+02  
 \*\* AL2CU\_C16  
 LIQUID  
 Calculated. 3 equilibria  
 Terminating at known equilibrium

Phase region boundary 13 at: 6.069E-02 8.026E+02  
 \*\* AL2CU\_C16  
 DIAMOND\_A4  
 LIQUID  
 Calculated. 22 equilibria

Phase region boundary 14 at: 9.890E-02 8.509E+02  
 \*\* AL2CU\_C16  
 \*\* ALCU\_ETA  
 DIAMOND\_A4  
 LIQUID

Phase region boundary 15 at: 1.058E-01 8.509E+02  
 AL2CU\_C16  
 \*\* ALCU\_ETA  
 DIAMOND\_A4

Phase region boundary 16 at: 1.350E-01 8.509E+02  
 \*\* AL2CU\_C16  
 ALCU\_ETA  
 DIAMOND\_A4

Phase region boundary 17 at: 1.058E-01 8.509E+02  
 AL2CU\_C16  
 DIAMOND\_A4  
 \*\* LIQUID

Phase region boundary 18 at: 1.350E-01 8.509E+02  
 ALCU\_ETA  
 DIAMOND\_A4  
 \*\* LIQUID

Phase region boundary 19 at: 9.890E-02 8.509E+02  
 \*\* ALCU\_ETA  
 DIAMOND\_A4  
 LIQUID  
 Calculated.. 2 equilibria  
 Terminating at axis limit.

Phase region boundary 20 at: 1.581E-02 7.950E+02  
 \*\* AL2CU\_C16  
 FCC\_L12  
 LIQUID  
 Calculated. 18 equilibria  
 Terminating at known equilibrium

Phase region boundary 21 at: 1.147E-02 7.950E+02  
 DIAMOND\_A4  
 FCC\_L12  
 \*\* LIQUID  
 Calculated. 2 equilibria

Phase region boundary 22 at: 1.107E-02 7.962E+02  
 \*\* DIAMOND\_A4  
 FCC\_L12  
 \*\* LIQUID

Phase region boundary 23 at: 1.107E-02 7.962E+02  
 FCC\_L12  
 \*\* LIQUID  
 Calculated 24 equilibria

Phase region boundary 24 at: 1.107E-02 7.962E+02  
 \*\* DIAMOND\_A4  
 FCC\_L12  
 Calculated.. 31 equilibria  
 Terminating at axis limit.

Phase region boundary 25 at: 1.107E-02 7.962E+02  
 \*\* DIAMOND\_A4  
 FCC\_L12  
 LIQUID  
 Calculated. 3 equilibria  
 Terminating at known equilibrium

Phase region boundary 26 at: 5.713E-02 7.965E+02  
 \*\* FCC\_L12  
 LIQUID  
 Calculated 43 equilibria

Phase region boundary 27 at: 5.000E-02 8.204E+02  
 \*\* FCC\_L12  
 LIQUID

```

Calculated                      37  equilibria

Phase region boundary  28 at:    5.000E-02  8.204E+02
** FCC_L12
LIQUID
Calculated.              4  equilibria
Terminating at known equilibrium

Phase region boundary  29 at:    5.000E-02  8.204E+02
** FCC_L12
LIQUID
Calculated              37  equilibria

Phase region boundary  30 at:    5.000E-02  8.204E+02
** FCC_L12
LIQUID
Calculated.              4  equilibria
Terminating at known equilibrium

Phase region boundary  31 at:    5.000E-02  8.204E+02
** FCC_L12
LIQUID
Calculated              37  equilibria

Phase region boundary  32 at:    5.000E-02  8.204E+02
** FCC_L12
LIQUID
Calculated.              4  equilibria
Terminating at known equilibrium

Phase region boundary  33 at:    5.000E-02  8.204E+02
** FCC_L12
LIQUID
Calculated              37  equilibria

Phase region boundary  34 at:    5.000E-02  8.204E+02
** FCC_L12
LIQUID
Calculated.              4  equilibria
Terminating at known equilibrium

Phase region boundary  35 at:    5.000E-02  8.204E+02
** FCC_L12
LIQUID
Calculated              37  equilibria

Phase region boundary  36 at:    5.000E-02  8.204E+02
** FCC_L12
LIQUID
Calculated.              4  equilibria
Terminating at known equilibrium

Phase region boundary  37 at:    5.000E-02  8.204E+02
** FCC_L12
LIQUID
Calculated              37  equilibria

Phase region boundary  38 at:    5.000E-02  8.204E+02
** FCC_L12
LIQUID
Calculated.              4  equilibria
Terminating at known equilibrium

Phase region boundary  39 at:    5.000E-02  8.204E+02
** FCC_L12
LIQUID
Calculated              37  equilibria

Phase region boundary  40 at:    5.000E-02  8.204E+02
** FCC_L12
LIQUID
Calculated.              4  equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex05\tcex
05.POLY3
CPU time for mapping                      9  seconds
POLY_3:
POLY_3: post

```

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-lab

... the command in full is SET\_LABEL\_CURVE\_OPTION

CURVE LABEL OPTION (A, B, C, D, E, F OR N) /N/: b

POST:

POST:

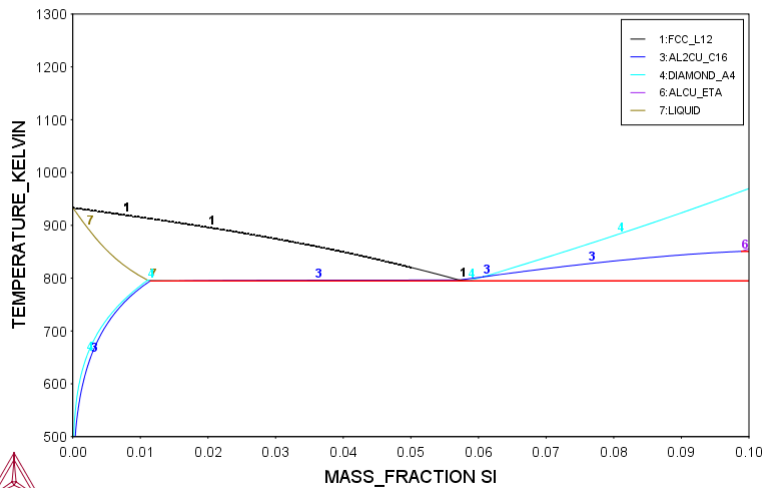
POST: set-title example 5a

POST: plot

... the command in full is PLOT\_DIAGRAM

# example 5a

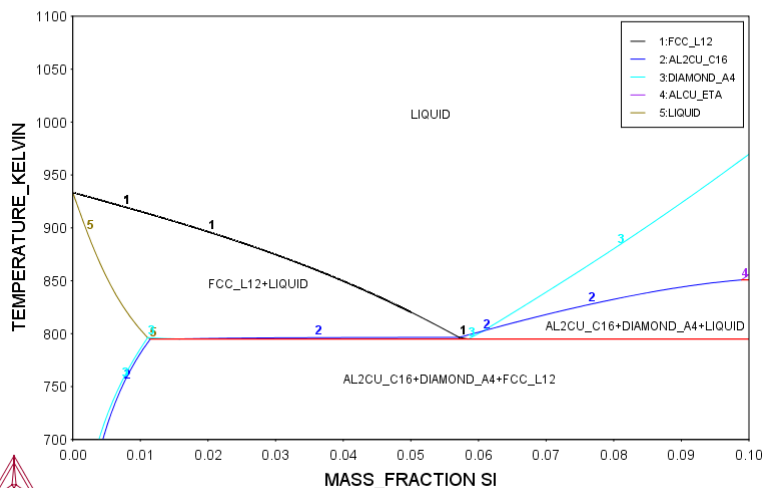
2016.05.16.13.07.33  
ALDEMO: AL, CU, SI  
P=1E5, N=1, X(CU)-2\*X(SI)=0



```
POST:
POST:@?<Hit_return_to_continue>
POST: s-s y n 700 1100
... the command in full is SET_SCALING_STATUS
POST: @@ Note that the three-phase region LIQ-Si-Al2Cu is an area and not
POST: @@ a single line as in a binary system. This is called a pseudo-binary section
POST: add .05 1000
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Stable phases are: LIQUID
Text size: /.36/:
POST: add .02 840
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Testing POLY result by global minimization procedure
Calculated 16528 grid points in 0 s
Stable phases are: FCC_L12+LIQUID
Text size: /.36/:
POST: add .04 750
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Testing POLY result by global minimization procedure
Calculated 16528 grid points in 0 s
Stable phases are: AL2CU_C16+DIAMOND_A4+FCC_L12
Text size: /.36/:
POST: add .07 800
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Testing POLY result by global minimization procedure
Calculated 16528 grid points in 0 s
Stable phases are: AL2CU_C16+DIAMOND_A4+LIQUID
Text size: /.36/:
POST:
POST: set-title example 5b
POST: plot
... the command in full is PLOT DIAGRAM
```

# example 5b

2016.05.16.13.07.35  
ALDEMO: AL, CU, SI  
P=1E5, N=1, X(CU)-2\*X(SI)=0



```
POST:
POST:@?<Hit_return_to_continue>
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex06

```
SYS>AboutSYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex06\tcex06.TCM"SYS: set-echo
SYS: @@
SYS: @@ Calculation of an isopleth in low alloyed
SYS: @@ Fe-Mn-Si-Cr-Ni-C steel. Calculation of a
SYS: @@ multicomponent phase diagram.
SYS: @@
SYS: set-log ex06,,
SYS: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3: @@ we use the define-material command in POLY and the TCFE steel database
POLY_3: @@ The material contains 1.5 %Cr + 0.4 %Mn + 3.5 %Ni + 0.3 %Si and 1 %C
POLY_3: @@ (by weight). These conditions are set by the command and in
POLY_3: @@ addition the temperature. Hidden commands set the pressure to 1 bar
POLY_3: @@ and that iron is "the rest".
POLY_3: @@ After calculating the first equilibrium we calculate a phase diagram
POLY_3: @@ with one axis variable as temperature and the other as the
POLY_3: @@ carbon content
POLY_3: def-mat
... the command in full is DEFINE_MATERIAL
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
L12_FCC B2_BCC B2_VACANCY
HIGH_SIGMA DICTRA_FCC_A1 REJECTED
Database /TCFE8/: tcfe7
Current database: Steels/Fe-Alloys v7.0

VA DEFINED
L12_FCC B2_BCC B2_VACANCY
HIGH_SIGMA DICTRA_FCC_A1 REJECTED
Major element or alloy: ?

Major element or alloy

The material must have a "major" element, usually the element which is
present in the largest amount. The fraction of this element will not be
set but be "the rest".

In some databases there are the "alloys" predefined. An alloy has a
default major element and have limits of the amounts of the alloying
elements. If the user stays within there limits the calculation should
give reasonable results.

Major element or alloy: fe
Composition input in mass (weight) percent? /Y/: y
1st alloying element: c
Mass (weight) percent /1/: 1
2nd alloying element: si .3
Next alloying element: mn .4
Next alloying element: ni 3.5
Next alloying element: cr 1.5
Next alloying element:
Temperature (C) /1000/: 1000
VA DEFINED
L12_FCC B2_BCC B2_VACANCY
HIGH_SIGMA DICTRA_FCC_A1 REJECTED
REINITIATING GES5 .....
... the command in full is DEFINE_ELEMENTS
FE DEFINED
... the command in full is DEFINE_ELEMENTS
C DEFINED
... the command in full is DEFINE_ELEMENTS
SI DEFINED
... the command in full is DEFINE_ELEMENTS
MN DEFINED
... the command in full is DEFINE_ELEMENTS
NI DEFINED
... the command in full is DEFINE_ELEMENTS
CR DEFINED

This database has following phases for the defined system

GAS:G LIQUID:L BCC_A2
FCC_A1 HCP_A3 DIAMOND_FCC_A4
GRAPHITE CEMENTITE M23C6
M7C3 M5C2 M3C2
KSI_CARBIDE A1_KAPPA KAPPA
FE4N_LP1 FECN_CHI SIGMA
CHI_A12 LAVES_PHASE_C14 M3SI
G_PHASE CR3SI FE2SI
MSI M5SI3 NBNI3
NI3TI AL4C3 FE8SI2C
SIC

Reject phase(s) /NONE/: NONE
Restore phase(s): /NONE/: NONE

.....

The following phases are retained in this system:

GAS:G LIQUID:L BCC_A2
FCC_A1 HCP_A3 DIAMOND_FCC_A4
GRAPHITE CEMENTITE M23C6
M7C3 M5C2 M3C2
KSI_CARBIDE A1_KAPPA KAPPA
FE4N_LP1 FECN_CHI SIGMA
CHI_A12 LAVES_PHASE_C14 M3SI
G_PHASE CR3SI FE2SI
MSI M5SI3 NBNI3
NI3TI AL4C3 FE8SI2C
SIC

.....

OK? /Y/: Y
```



```

ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

```

#### List of references for assessed data

```

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-OK-

```

Should any phase have a miscibility gap check? /N/: N

```

Using global minimization procedure
Calculated          23376 grid points in          1 s
Found the set of lowest grid points in          0 s
Calculated POLY solution          0 s, total time    1 s

```

POLY\_3:

POLY\_3: 1-e

... the command in full is LIST\_EQUILIBRIUM

OUTPUT TO SCREEN OR FILE /SCREEN/:

Options /VWCS/: VWCS

Output from POLY-3, equilibrium = 1, label A0 , database: TCFe7

Conditions:

T=1273.15, W(C)=1E-2, W(SI)=3E-3, W(MN)=4E-3, W(NI)=3.5E-2, W(CR)=1.5E-2,  
P=1E5, N=1

DEGREES OF FREEDOM 0

Temperature 1273.15 K ( 1000.00 C), Pressure 1.000000E+05

Number of moles of components 1.00000E+00, Mass in grams 5.37536E+01

Total Gibbs energy -6.46529E+04, Enthalpy 3.76283E+04, Volume 7.13756E-06

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
C	4.4754E-02	1.0000E-02	8.3878E-02	-2.6235E+04	SER
CR	1.5507E-02	1.5000E-02	1.2598E-04	-9.5052E+04	SER
FE	8.9803E-01	9.3300E-01	2.4771E-03	-6.3521E+04	SER
MN	3.9138E-03	4.0000E-03	3.0765E-06	-1.3435E+05	SER
NI	3.2056E-02	3.5000E-02	6.1631E-05	-1.0262E+05	SER
SI	5.7417E-03	3.0000E-03	6.4662E-09	-1.9961E+05	SER

FCC\_A1 Status ENTERED Driving force 0.0000E+00

Moles 1.0000E+00, Mass 5.3754E+01, Volume fraction 1.0000E+00 Mass fractions:

FE 9.3300E-01 CR 1.5000E-02 MN 4.0000E-03

NI 3.5000E-02 C 1.0000E-02 SI 3.0000E-03

POLY\_3:Hit RETURN to continue

POLY\_3: @@ Note that values now must be set in fractions and Kelvin!

POLY\_3: @@ Sorry about that

POLY\_3: s-a-v 1 w(c)

... the command in full is SET\_AXIS\_VARIABLE

Min value /0/: 0

Max value /1/: .01

Increment /2.5E-04/: 1E-4

POLY\_3: s-a-v 2 t

... the command in full is SET\_AXIS\_VARIABLE

Min value /0/: 700

Max value /1/: 1300

Increment /15/:

POLY\_3: save tcex06 y

... the command in full is SAVE\_WORKSPACES

POLY\_3: map

Version S mapping is selected

Generating start equilibrium 1

Generating start equilibrium 2

Generating start equilibrium 3

Generating start equilibrium 4

Generating start equilibrium 5

Generating start equilibrium 6

Generating start equilibrium 7

Generating start equilibrium 8

Generating start equilibrium 9

Generating start equilibrium 10

Generating start equilibrium 11

Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Tie-lines not in the plane of calculation

Generating start point 1

Generating start point 2

Generating start point 3

Generating start point 4

Generating start point 5

Generating start point 6

Generating start point 7

Generating start point 8

Generating start point 9

Generating start point 10

Working hard

Generating start point 11

Generating start point 12

Generating start point 13

Generating start point 14

Generating start point 15

Generating start point 16

Generating start point 17

Generating start point 18

Generating start point 19

Generating start point 20

Working hard

Generating start point 21

Generating start point 22

Generating start point 23

Generating start point 24

Generating start point 25

Generating start point 26

Generating start point 27

Generating start point 28

Phase region boundary 1 at: 1.953E-03 7.100E+02

BCC\_A2

FCC\_A1

\*\* M3C2

M7C3

Calculated.. 3 equilibria

Terminating at axis limit.

Phase region boundary 2 at: 1.810E-03 7.000E+02

BCC\_A2

FCC\_A1

\*\* M3C2

M7C3

Calculated.. 10 equilibria

Phase region boundary 3 at: 2.222E-03 7.146E+02

BCC\_A2

FCC\_A1

\*\* GRAPHITE

\*\* M3C2

M7C3

Phase region boundary 4 at: 2.222E-03 7.146E+02

BCC\_A2

FCC\_A1

GRAPHITE

```

** M3C2
M7C3
Calculated..                80 equilibria
Terminating at axis limit.

Phase region boundary  5 at:  2.222E-03  7.146E+02
  BCC_A2
  FCC_A1
** GRAPHITE
M7C3
Calculated..                21 equilibria

Phase region boundary  6 at:  2.784E-03  8.955E+02
  BCC_A2
** CEMENTITE
  FCC_A1
** GRAPHITE
M7C3

Phase region boundary  7 at:  2.784E-03  8.955E+02
  BCC_A2
  CEMENTITE
  FCC_A1
** GRAPHITE
M7C3
Calculated..                28 equilibria

Phase region boundary  8 at:  5.463E-03  8.990E+02
  BCC_A2
  CEMENTITE
  FCC_A1
** GRAPHITE
** M7C3

Phase region boundary  9 at:  5.463E-03  8.990E+02
  BCC_A2
  CEMENTITE
  FCC_A1
** GRAPHITE
Calculated..                48 equilibria
Terminating at axis limit.

Phase region boundary 10 at:  5.463E-03  8.990E+02
  BCC_A2
  CEMENTITE
  FCC_A1
** M7C3
Calculated..                22 equilibria

Phase region boundary 11 at:  6.268E-03  9.872E+02
** BCC_A2
  CEMENTITE
  FCC_A1
** M7C3

Phase region boundary 12 at:  6.268E-03  9.872E+02
  CEMENTITE
  FCC_A1
** M7C3
Calculated..                8 equilibria

Phase region boundary 13 at:  6.107E-03  1.088E+03
** CEMENTITE
  FCC_A1
** M7C3

Phase region boundary 14 at:  6.107E-03  1.088E+03
  FCC_A1
** M7C3
Calculated..                34 equilibria

Phase region boundary 15 at:  2.846E-03  1.004E+03
** BCC_A2
  FCC_A1
** M7C3

Phase region boundary 16 at:  2.846E-03  1.004E+03
  BCC_A2
  FCC_A1
** M7C3
Calculated..                53 equilibria
Terminating at axis limit.

Phase region boundary 17 at:  2.846E-03  1.004E+03
** BCC_A2
  FCC_A1
Calculated..                41 equilibria

Phase region boundary 18 at:  2.846E-03  1.004E+03
** BCC_A2
  FCC_A1
M7C3
Calculated..                26 equilibria

Phase region boundary 19 at:  5.334E-03  9.878E+02
** BCC_A2
** CEMENTITE
  FCC_A1
M7C3

Phase region boundary 20 at:  5.334E-03  9.878E+02
** BCC_A2
  CEMENTITE
  FCC_A1
M7C3
Calculated..                11 equilibria
Terminating at known equilibrium

Phase region boundary 21 at:  5.334E-03  9.878E+02
** CEMENTITE
  FCC_A1
M7C3
Calculated..                13 equilibria
Terminating at known equilibrium

Phase region boundary 22 at:  5.334E-03  9.878E+02

```

```

    BCC_A2
** CEMENTITE
    FCC_A1
    M7C3
Calculated.                36 equilibria
Terminating at known equilibrium

Phase region boundary 23 at:  6.107E-03  1.088E+03
** CEMENTITE
    FCC_A1
Calculated..                41 equilibria
Terminating at axis limit.

Phase region boundary 24 at:  6.268E-03  9.872E+02
** BCC_A2
    CEMENTITE
    FCC_A1
Calculated..                40 equilibria
Terminating at axis limit.

Phase region boundary 25 at:  5.463E-03  8.990E+02
    BCC_A2
    CEMENTITE
    FCC_A1
    GRAPHITE
** M7C3
Calculated..                48 equilibria
Terminating at axis limit.

Phase region boundary 26 at:  2.784E-03  8.955E+02
    BCC_A2
** CEMENTITE
    FCC_A1
    GRAPHITE
    M7C3
Calculated..                75 equilibria
Terminating at axis limit.

Phase region boundary 27 at:  2.222E-03  7.146E+02
    BCC_A2
    FCC_A1
** GRAPHITE
    M3C2
    M7C3
Calculated.                 2 equilibria

Phase region boundary 28 at:  2.164E-03  7.078E+02
    BCC_A2
    FCC_A1
** GRAPHITE
    M3C2
** M7C3

Phase region boundary 29 at:  2.164E-03  7.078E+02
    BCC_A2
    FCC_A1
** GRAPHITE
    M3C2
Calculated..                2 equilibria
Terminating at axis limit.

Phase region boundary 30 at:  2.164E-03  7.078E+02
    BCC_A2
    FCC_A1
    M3C2
** M7C3
Calculated..                16 equilibria
Terminating at axis limit.

Phase region boundary 31 at:  2.164E-03  7.078E+02
    BCC_A2
    FCC_A1
    GRAPHITE
    M3C2
** M7C3
Calculated..                81 equilibria
Terminating at axis limit.

Phase region boundary 32 at:  1.953E-03  7.100E+02
    BCC_A2
    FCC_A1
** M3C2
    M7C3
Calculated.                 7 equilibria
Terminating at known equilibrium

Phase region boundary 33 at:  1.000E-04  9.417E+02
    BCC_A2
    FCC_A1
** M7C3
Calculated..                26 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 34 at:  1.000E-04  9.417E+02
    BCC_A2
    FCC_A1
** M7C3
Calculated.                 29 equilibria
Terminating at known equilibrium

Phase region boundary 35 at:  3.367E-03  7.146E+02
    BCC_A2
    FCC_A1
    GRAPHITE
** M3C2
    M7C3
Calculated.                 13 equilibria
Terminating at known equilibrium

Phase region boundary 36 at:  3.367E-03  7.146E+02
    BCC_A2
    FCC_A1
    GRAPHITE
** M3C2
    M7C3

```

Calculated.. 69 equilibria  
Terminating at known equilibrium  
Terminating at axis limit.

Phase region boundary 37 at: 6.633E-03 7.147E+02  
BCC\_A2  
FCC\_A1  
GRAPHITE  
\*\* M3C2  
M7C3

Calculated.. 46 equilibria  
Terminating at known equilibrium

Phase region boundary 38 at: 6.633E-03 7.147E+02  
BCC\_A2  
FCC\_A1  
GRAPHITE  
\*\* M3C2  
M7C3

Calculated.. 36 equilibria  
Terminating at known equilibrium  
Terminating at axis limit.

Phase region boundary 39 at: 2.185E-03 7.100E+02  
BCC\_A2  
FCC\_A1  
\*\* GRAPHITE  
M3C2  
M7C3

Calculated.. 2 equilibria  
Terminating at known equilibrium

Phase region boundary 40 at: 2.185E-03 7.100E+02  
BCC\_A2  
FCC\_A1  
\*\* GRAPHITE  
M3C2  
M7C3

Calculated.. 2 equilibria  
Terminating at known equilibrium

Phase region boundary 41 at: 9.900E-03 7.148E+02  
BCC\_A2  
FCC\_A1  
GRAPHITE  
\*\* M3C2  
M7C3

Calculated.. 78 equilibria  
Terminating at known equilibrium

Phase region boundary 42 at: 9.900E-03 7.148E+02  
BCC\_A2  
FCC\_A1  
GRAPHITE  
\*\* M3C2  
M7C3

Calculated.. 3 equilibria  
Terminating at known equilibrium  
Terminating at axis limit.

Phase region boundary 43 at: 2.772E-03 9.033E+02  
BCC\_A2  
\*\* CEMENTITE  
FCC\_A1  
M7C3

Calculated.. 2 equilibria  
Terminating at known equilibrium

Phase region boundary 44 at: 2.772E-03 9.033E+02  
BCC\_A2  
\*\* CEMENTITE  
FCC\_A1  
M7C3

Calculated.. 32 equilibria  
Terminating at known equilibrium

Phase region boundary 45 at: 5.632E-03 9.033E+02  
BCC\_A2  
CEMENTITE  
FCC\_A1  
\*\* GRAPHITE

Calculated.. 3 equilibria  
Terminating at known equilibrium

Phase region boundary 46 at: 5.632E-03 9.033E+02  
BCC\_A2  
CEMENTITE  
FCC\_A1  
\*\* GRAPHITE

Calculated.. 46 equilibria  
Terminating at known equilibrium  
Terminating at axis limit.

Phase region boundary 47 at: 6.376E-03 1.097E+03  
\*\* CEMENTITE  
FCC\_A1

Calculated.. 4 equilibria  
Terminating at known equilibrium

Phase region boundary 48 at: 6.376E-03 1.097E+03  
\*\* CEMENTITE  
FCC\_A1

Calculated.. 39 equilibria  
Terminating at known equilibrium  
Terminating at axis limit.

Phase region boundary 49 at: 6.376E-03 1.097E+03  
\*\* CEMENTITE  
FCC\_A1

Calculated.. 4 equilibria  
Terminating at known equilibrium

Phase region boundary 50 at: 6.376E-03 1.097E+03  
\*\* CEMENTITE  
FCC\_A1

Calculated.. 39 equilibria

```

Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 51 at: 1.000E-04 1.051E+03
** BCC_A2
FCC_A1
Calculated 4 equilibria

Phase region boundary 52 at: 1.000E-04 1.051E+03
** BCC_A2
FCC_A1
Calculated. 29 equilibria
Terminating at known equilibrium

Phase region boundary 53 at: 3.367E-03 1.020E+03
FCC_A1
** M7C3
Calculated. 7 equilibria
Terminating at known equilibrium

Phase region boundary 54 at: 3.367E-03 1.020E+03
FCC_A1
** M7C3
Calculated. 29 equilibria
Terminating at known equilibrium

Phase region boundary 55 at: 6.633E-03 1.105E+03
** CEMENTITE
FCC_A1
Calculated. 7 equilibria
Terminating at known equilibrium

Phase region boundary 56 at: 6.633E-03 1.105E+03
** CEMENTITE
FCC_A1
Calculated.. 36 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 57 at: 9.900E-03 1.198E+03
** CEMENTITE
FCC_A1
Calculated. 39 equilibria
Terminating at known equilibrium

Phase region boundary 58 at: 9.900E-03 1.198E+03
** CEMENTITE
FCC_A1
Calculated.. 4 equilibria
Terminating at known equilibrium
Terminating at axis limit.
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex06\tcex
06.POLY3
CPU time for mapping 34 seconds
POLY_3: post

```

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

```

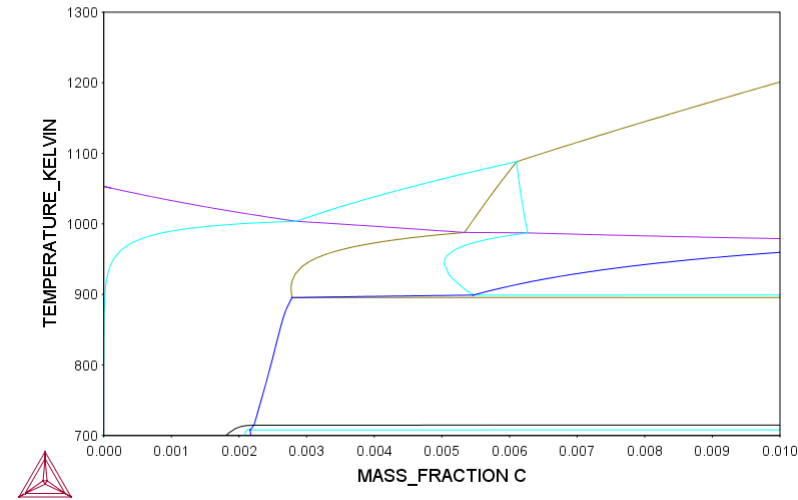
POST:
POST:
POST: set-title example 6a
POST: plot
... the command in full is PLOT DIAGRAM
                                example 6a

```

```

2016.05.16.13.10.27
TCFE7: C, CR, FE, MN, NI, SI
W(SI)=3E-3, W(MN)=4E-3, W(NI)=3.5E-2, W(CR)=1.5E-2, P=1E5, N=1

```



```

POST:
POST:Hit RETURN to continue
POST: @@ Use more practical quantities in the plot and
POST: @@ label the curves
POST: s-d-a x w-p c
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t-c
... the command in full is SET_DIAGRAM_AXIS
POST: s-s x n 0 1
... the command in full is SET_SCALING_STATUS
POST:
POST: s-s y n 600 900
... the command in full is SET_SCALING_STATUS
POST:
POST: s-lab b

```

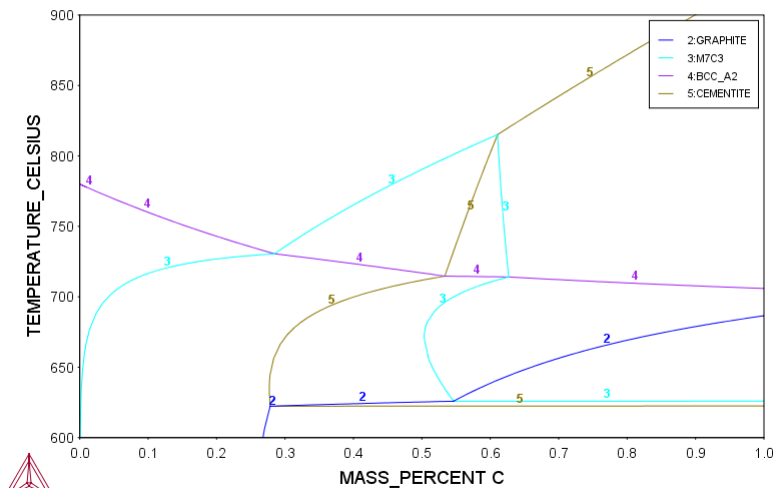
```
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 6b
POST:
POST: plot
... the command in full is PLOT DIAGRAM
```

#### example 6b

2016.05.16.13.10.29

TCFE7: C, CR, FE, MN, NI, SI

W(SI)=3E-3, W(MN)=4E-3, W(NI)=3.5E-2, W(CR)=1.5E-2, P=1E5, N=1



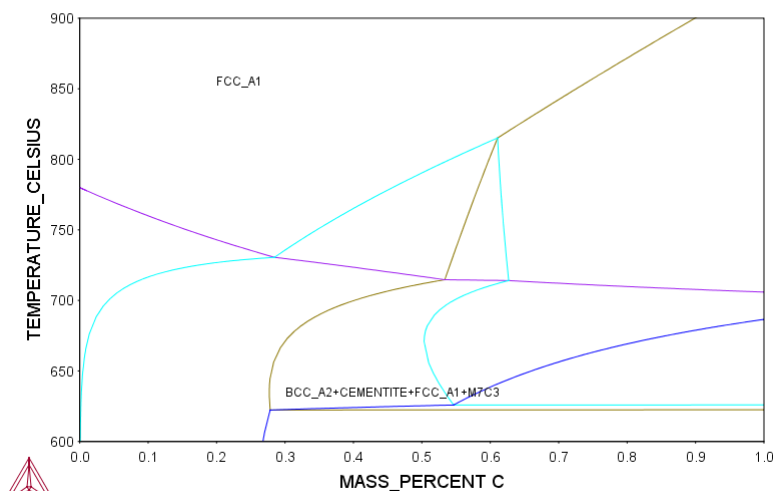
```
POST:
POST:Hit RETURN to continue
POST: @@ Determine the phase region at the iron rich side
POST: add .2 850
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Calculated 23376 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
Stable phases are: FCC_A1
Text size: /.36/:
POST: @@ Knowing that only FCC (or austenite) is stable in that region and
POST: @@ which phase is stable along each line, one can determine the phases
POST: @@ in each region. For example at 0.3 % C and 630 degree C one should
POST: @@ have FCC+BCC+M7C3+CEMENTITE.
POST: @@ Check by adding a label
POST: add .3 630
... the command in full is ADD_LABEL_TEXT
Automatic phase labels? /Y/:
Automatic labelling not always possible
Using global minimization procedure
Calculated 23376 grid points in 1 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 1 s
Stable phases are: BCC_A2+CEMENTITE+FCC_A1+M7C3
Text size: /.36/:
POST: s-lab n
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 6c
POST:
POST: plot
... the command in full is PLOT DIAGRAM
```

#### example 6c

2016.05.16.13.10.32

TCFE7: C, CR, FE, MN, NI, SI

W(SI)=3E-3, W(MN)=4E-3, W(NI)=3.5E-2, W(CR)=1.5E-2, P=1E5, N=1



```
POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex07

About Stockholm, Sweden

Software (build 9533) running on WinNT 64-bit wordlength  
Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118  
License library version: 8.5.1.0017  
Linked: Mon May 16 09:31:44 2016

SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex07\tcex07.TCM"SYS: set-echo

SYS: @@  
SYS: @@ Calculation  
SYS: @@ of single equilibria in low alloyed  
SYS: @@ Fe-Mn-Si-Cr-Ni-C steel.  
SYS: @@  
SYS: @@ Single equilibrium calculations in a steel.  
SYS: @@  
SYS: @@ There are two common ways to perform a single equilibrium calculation.  
SYS: @@ 1) start from scratch: firstly get data from database, then in  
SYS: @@ POLY use SET\_CONDITION and COMPUTE\_EQUILIBRIUM.  
SYS: @@ 2) Go directly to POLY, and use DEFINE\_MATERIAL.  
SYS: @@  
SYS: @@ One often wants to know the temperature or composition where one phase  
SYS: @@ forms or disappears, COMPUTE\_TRANSITION is a useful command. It is the  
SYS: @@ same as the CHANGE\_STATUS/SET\_CONDITION/COMPUTE\_EQUILIBRIUM combination.  
SYS: @@  
SYS: set-log ex07,,  
SYS: @@ The alloy composition is 1 wt% Cr, 0.3 wt% Si, 0.3wt% Mn,  
SYS: @@ 2.8 wt% Ni and 0.55 wt% C  
SYS: go p-3  
... the command in full is GOTO\_MODULE

POLY version 3.32  
POLY\_3: def-mat  
... the command in full is DEFINE\_MATERIAL  
THERMODYNAMIC DATABASE module  
Current database: Steels/Fe-Alloys v8.0

VA DEFINED  
L12\_FCC B2\_BCC B2\_VACANCY  
HIGH\_SIGMA DICTRA\_FCC\_A1 REJECTED  
Database /TCFE8/: tcfe7  
Current database: Steels/Fe-Alloys v7.0

VA DEFINED  
L12\_FCC B2\_BCC B2\_VACANCY  
HIGH\_SIGMA DICTRA\_FCC\_A1 REJECTED  
Major element or alloy: fe  
Composition input in mass (weight) percent? /Y/:  
1st alloying element: c .55  
2nd alloying element: cr 1  
Next alloying element: mn .3 ni 2.8 si .3  
Next alloying element:  
Temperature (C) /1000/: 600

VA DEFINED  
L12\_FCC B2\_BCC B2\_VACANCY  
HIGH\_SIGMA DICTRA\_FCC\_A1 REJECTED  
REINITIATING GES5 .....  
... the command in full is DEFINE\_ELEMENTS  
FE DEFINED  
... the command in full is DEFINE\_ELEMENTS  
C DEFINED  
... the command in full is DEFINE\_ELEMENTS  
CR DEFINED  
... the command in full is DEFINE\_ELEMENTS  
MN DEFINED  
... the command in full is DEFINE\_ELEMENTS  
NI DEFINED  
... the command in full is DEFINE\_ELEMENTS  
SI DEFINED

This database has following phases for the defined system

GAS:G	LIQUID:L	BCC_A2
FCC_A1	HCP_A3	DIAMOND_FCC_A4
GRAPHITE	CEMENTITE	M23C6
M7C3	M5C2	M3C2
KSI_CARBIDE	A1_KAPPA	KAPPA
FE4N_LP1	FECN_CHI	SIGMA
CHI_A12	LAVES_PHASE_C14	M3SI
G_PHASE	CR3SI	FE2SI
MSI	M5SI3	NBNI3
NI3TI	AL4C3	FE8SI2C
SIC		

Reject phase(s) /NONE/:  
Restore phase(s) : /NONE/:

.....  
The following phases are retained in this system:

GAS:G	LIQUID:L	BCC_A2
FCC_A1	HCP_A3	DIAMOND_FCC_A4
GRAPHITE	CEMENTITE	M23C6
M7C3	M5C2	M3C2
KSI_CARBIDE	A1_KAPPA	KAPPA
FE4N_LP1	FECN_CHI	SIGMA
CHI_A12	LAVES_PHASE_C14	M3SI
G_PHASE	CR3SI	FE2SI
MSI	M5SI3	NBNI3
NI3TI	AL4C3	FE8SI2C
SIC		

.....  
OK? /Y/: Y  
ELEMENTS .....  
SPECIES .....  
PHASES .....  
... the command in full is AMEND\_PHASE\_DESCRIPTION



```

... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

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-OK-

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```

Should any phase have a miscibility gap check? /N/: N
Using global minimization procedure
Calculated          23376 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution          0 s, total time          0 s
POLY_3:
POLY_3: @@ The first equilibrium is calculated automatically
POLY_3: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
Output from POLY-3, equilibrium =          1, label A0 , database: TCFE7

Conditions:

```

T=873.15, W(C)=5.5E-3, W(CR)=1E-2, W(MN)=3E-3, W(NI)=2.8E-2, W(SI)=3E-3,  
P=1E5, N=1  
DEGREES OF FREEDOM 0

Temperature 873.15 K ( 600.00 C), Pressure 1.000000E+05  
Number of moles of components 1.00000E+00, Mass in grams 5.46196E+01  
Total Gibbs energy -3.56732E+04, Enthalpy 1.79282E+04, Volume 7.20787E-06

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
C	2.5011E-02	5.5000E-03	2.6153E-01	-9.7369E+03	SER
CR	1.0505E-02	1.0000E-02	2.4479E-04	-6.0366E+04	SER
FE	9.2961E-01	9.5050E-01	8.6789E-03	-3.4461E+04	SER
MN	2.9826E-03	3.0000E-03	2.8925E-05	-7.5871E+04	SER
NI	2.6058E-02	2.8000E-02	3.4662E-04	-5.7841E+04	SER
SI	5.8342E-03	3.0000E-03	2.9885E-11	-1.7593E+05	SER

BCC\_A2 Status ENTERED Driving force 0.0000E+00  
Moles 9.5814E-01, Mass 5.3405E+01, Volume fraction 9.6729E-01 Mass fractions:  
FE 9.63504E-01 SI 3.06820E-03 MN 2.28601E-03  
NI 2.85952E-02 CR 2.52703E-03 C 1.97123E-05

M7C3 Status ENTERED Driving force 0.0000E+00  
Moles 2.4194E-02, Mass 1.0019E+00, Volume fraction 1.9532E-02 Mass fractions:  
FE 4.58650E-01 C 8.70086E-02 NI 2.20485E-03  
CR 4.10444E-01 MN 4.16928E-02 SI 3.04624E-12

GRAPHITE Status ENTERED Driving force 0.0000E+00  
Moles 1.7665E-02, Mass 2.1218E-01, Volume fraction 1.3181E-02 Mass fractions:  
C 1.00000E+00 NI 0.00000E+00 FE 0.00000E+00  
SI 0.00000E+00 MN 0.00000E+00 CR 0.00000E+00

POLY\_3: ?

... the command in full is HELP  
ADD\_INITIAL\_EQUILIBRIUM EXIT REINITIATE\_MODULE  
ADVANCED\_OPTIONS GOTO\_MODULE SAVE\_WORKSPACES  
AMEND\_STORED\_EQUILIBRIA HELP SELECT\_EQUILIBRIUM  
BACK INFORMATION SET\_ALL\_START\_VALUES  
CHANGE\_STATUS LIST\_AXIS\_VARIABLE SET\_AXIS\_VARIABLE  
COMPUTE\_EQUILIBRIUM LIST\_CONDITIONS SET\_CONDITION  
COMPUTE\_TRANSITION LIST\_EQUILIBRIUM SET\_INPUT\_AMOUNTS  
CREATE\_NEW\_EQUILIBRIUM LIST\_INITIAL\_EQUILIBRIA SET\_INTERACTIVE  
DEFINE\_COMPONENTS LIST\_STATUS SET\_NUMERICAL\_LIMITS  
DEFINE\_DIAGRAM LIST\_SYMBOLS SET\_REFERENCE\_STATE  
DEFINE\_MATERIAL LOAD\_INITIAL\_EQUILIBRIUM SET\_START\_CONSTITUITION  
DELETE\_INITIAL\_EQUILIB MACRO\_FILE\_OPEN SET\_START\_VALUE  
DELETE\_SYMBOL MAP SHOW\_VALUE  
ENTER\_SYMBOL POST STEP\_WITH\_OPTIONS  
EVALUATE\_FUNCTIONS READ\_WORKSPACES TABULATE

POLY\_3:Hit RETURN to continue

POLY\_3: @@ Increase Cr until all Graphite disappears. Calculate this

POLY\_3: @@ directly using the COMPUTE-TRANSITION command. You

POLY\_3: @@ must release the Cr content of course

POLY\_3: c-t

... the command in full is COMPUTE\_TRANSITION  
This command is a combination of CHANGE\_STATUS and SET\_CONDITION  
to calculate directly when a phase may form by releasing one condition.

Phase to form: grap

You must release one of these conditions  
T=873.15, W(C)=5.5E-3, W(CR)=1E-2, W(MN)=3E-3, W(NI)=2.8E-2, W(SI)=3E-3,  
P=1E5, N=1 DEGREES OF FREEDOM 0

Give the state variable to be removed /T/: w(cr)

Testing POLY result by global minimization procedure

Using already calculated grid

To form GRAP the condition is set to W(CR)=.0293768365613

POLY\_3: l-e

... the command in full is LIST\_EQUILIBRIUM

OUTPUT TO SCREEN OR FILE /SCREEN/:

Options /VWCS/: VWCS

Output from POLY-3, equilibrium = 1, label A0 , database: TCFE7

Conditions:

T=873.15, W(C)=5.5E-3, W(CR)=2.93768E-2, W(MN)=3E-3, W(NI)=2.8E-2,  
W(SI)=3E-3, P=1E5, N=1  
DEGREES OF FREEDOM 0

Temperature 873.15 K ( 600.00 C), Pressure 1.000000E+05  
Number of moles of components 1.00000E+00, Mass in grams 5.45430E+01  
Total Gibbs energy -3.61950E+04, Enthalpy 1.77828E+04, Volume 7.15532E-06

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
C	2.4976E-02	5.5000E-03	2.6153E-01	-9.7369E+03	SER
CR	3.0816E-02	2.9377E-02	2.5353E-04	-6.0112E+04	SER
FE	9.0938E-01	9.3112E-01	8.6730E-03	-3.4466E+04	SER
MN	2.9784E-03	3.0000E-03	1.8254E-05	-7.9213E+04	SER
NI	2.6022E-02	2.8000E-02	3.6127E-04	-5.7540E+04	SER
SI	5.8260E-03	3.0000E-03	3.1190E-11	-1.7562E+05	SER

BCC\_A2 Status ENTERED Driving force 0.0000E+00  
Moles 9.1702E-01, Mass 5.1110E+01, Volume fraction 9.3250E-01 Mass fractions:  
FE 9.62968E-01 SI 3.20151E-03 MN 1.45355E-03  
NI 2.97317E-02 CR 2.62575E-03 C 1.94050E-05

M7C3 Status ENTERED Driving force 0.0000E+00  
Moles 8.2978E-02, Mass 3.4330E+00, Volume fraction 6.7498E-02 Mass fractions:  
FE 4.57021E-01 C 8.70942E-02 NI 2.21880E-03  
CR 4.27642E-01 MN 2.60233E-02 SI 3.17758E-12

GRAPHITE Status ENTERED Driving force 0.0000E+00  
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:  
C 1.00000E+00 NI 0.00000E+00 FE 0.00000E+00  
SI 0.00000E+00 MN 0.00000E+00 CR 0.00000E+00

POLY\_3:Hit RETURN to continue

POLY\_3: @@ Graphite disappears when we have this chromium content 2.94 w/o

POLY\_3: @@ The amount of Cr can be obtain directly with a show command

POLY\_3: show w(cr)

... the command in full is SHOW\_VALUE

W(CR)=2.9376837E-2

POLY\_3: @@ This is automatically set as new condition by the C-T command

POLY\_3: @@ and the amount of graphite is zero.

POLY\_3: l-st ph

... the command in full is LIST\_STATUS

\*\*\* STATUS FOR ALL PHASES

PHASE	STATUS	DRIVING FORCE	MOLES
M7C3	ENTERED	0.000000E+00	8.297805E-02
GRAPHITE	ENTERED	0.000000E+00	0.000000E+00
BCC_A2	ENTERED	0.000000E+00	9.170220E-01

```

CEMENTITE          ENTERED      -1.684846E-02    0.000000E+00
FCC_A1             ENTERED      -1.785775E-02    0.000000E+00
FCC_A1#2           ENTERED      -1.785775E-02    0.000000E+00
M23C6              ENTERED      -9.187797E-02    0.000000E+00
KAPPA              ENTERED      -1.728791E-01    0.000000E+00
M3C2               ENTERED      -2.522305E-01    0.000000E+00
HCP_A3             ENTERED      -2.617842E-01    0.000000E+00
HCP_A3#2           ENTERED      -2.617842E-01    0.000000E+00
FECN_CHI           ENTERED      -3.867251E-01    0.000000E+00
M5C2               ENTERED      -5.597293E-01    0.000000E+00
ENTERED PHASES WITH DRIVING FORCE LESS THAN  -6.753681E-01
LIQUID SIGMA CHI A12 DIAMOND FCC_A4 FE4N LP1 LAVES PHASE_C14 KSI CARBIDE
FE8SI2C G PHASE M3SI NI3TI FE2SI NBNI3 CR3SI M5SI3 MSI SIC AL4C3 GAS
POLY_3: @@ Now determine the maximum temperature with no Austenite (FCC_A1),
POLY_3: @@ i.e. A1 temperature.
POLY_3: @@ We use again the new command COMPUTE-TRANSITION
POLY_3: c-t
... the command in full is COMPUTE_TRANSITION
This command is a combination of CHANGE_STATUS and SET_CONDITION
to calculate directly when a phase may form by releasing one condition.
Phase to form: fcc_a1
You must release one of these conditions
T=873.15, W(C)=5.5E-3, W(CR)=2.93768E-2, W(MN)=3E-3, W(NI)=2.8E-2,
W(SI)=3E-3, P=1E5, N=1 DEGREES OF FREEDOM 0
Give the state variable to be removed /T/: t
Testing POLY result by global minimization procedure
Calculated 23376 grid points in 0 s
To form FCC_A1 the condition is set to T=915.22062277
POLY_3: l-c
... the command in full is LIST_CONDITIONS
T=915.221, W(C)=5.5E-3, W(CR)=2.93768E-2, W(MN)=3E-3, W(NI)=2.8E-2,
W(SI)=3E-3, P=1E5, N=1 DEGREES OF FREEDOM 0
POLY_3: @@ This command does the same as the change-status/set-cond/compute-equil,
POLY_3: @@ Notice that the temperature is set back as condition with the new value.
POLY_3: @@ If we want temperatures in Celsius we can enter a function.
POLY_3: ent fun tc=t-273;
... the command in full is ENTER_SYMBOL
POLY_3: sh tc
... the command in full is SHOW_VALUE
TC=642.22062
POLY_3: Hit RETURN to continue
POLY_3:
POLY_3: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
Output from POLY-3, equilibrium = 1, label A0 , database: TCFE7

Conditions:
T=915.221, W(C)=5.5E-3, W(CR)=2.93768E-2, W(MN)=3E-3, W(NI)=2.8E-2,
W(SI)=3E-3, P=1E5, N=1
DEGREES OF FREEDOM 0

Temperature 915.22 K ( 642.07 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 5.45430E+01
Total Gibbs energy -3.88407E+04, Enthalpy 1.96981E+04, Volume 7.16989E-06

Component      Moles      W-Fraction  Activity   Potential  Ref.stat
C               2.4976E-02  5.5000E-03  2.1560E-01 -1.1676E+04 SER
CR              3.0816E-02  2.9377E-02  2.6256E-04 -6.2742E+04 SER
FE              9.0938E-01  9.3112E-01  7.6560E-03 -3.7076E+04 SER
MN              2.9784E-03  3.0000E-03  1.5918E-05 -8.4071E+04 SER
NI              2.6022E-02  2.8000E-02  2.9594E-04 -6.1831E+04 SER
SI              5.8260E-03  3.0000E-03  6.4895E-11 -1.7851E+05 SER

BCC_A2          Status ENTERED      Driving force 0.0000E+00
Moles 9.1724E-01, Mass 5.1116E+01, Volume fraction 9.3276E-01 Mass fractions:
FE 9.61872E-01 CR 3.48152E-03 MN 1.68770E-03
NI 2.97230E-02 SI 3.20115E-03 C 3.45703E-05

M7C3            Status ENTERED      Driving force 0.0000E+00
Moles 8.2763E-02, Mass 3.4273E+00, Volume fraction 6.7240E-02 Mass fractions:
FE 4.72522E-01 C 8.70137E-02 NI 2.30172E-03
CR 4.15590E-01 MN 2.25722E-02 SI 8.20561E-12

FCC_A1          Status ENTERED      Driving force 0.0000E+00
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
FE 8.68031E-01 MN 1.44441E-02 SI 4.18888E-03
NI 1.05328E-01 CR 5.51928E-03 C 2.48820E-03
POLY_3: l-st
... the command in full is LIST_STATUS
Option /CPS/: cps
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS      REF. STATE      T(K)            P(Pa)
VA              ENTERED      SER
C               ENTERED      SER
CR              ENTERED      SER
FE              ENTERED      SER
MN              ENTERED      SER
NI              ENTERED      SER
SI              ENTERED      SER
*** STATUS FOR ALL PHASES
PHASE          STATUS      DRIVING FORCE      MOLES
M7C3           ENTERED      0.000000E+00      8.276289E-02
FCC_A1         ENTERED      0.000000E+00      0.000000E+00
BCC_A2         ENTERED      0.000000E+00      9.172371E-01
FCC_A1#2       ENTERED      -5.216451E-09      0.000000E+00
CEMENTITE      ENTERED      -6.422721E-03      0.000000E+00
M23C6          ENTERED      -7.334991E-02      0.000000E+00
GRAPHITE       ENTERED      -1.327548E-01      0.000000E+00
KAPPA          ENTERED      -1.370531E-01      0.000000E+00
HCP_A3         ENTERED      -2.513814E-01      0.000000E+00
HCP_A3#2       ENTERED      -2.513814E-01      0.000000E+00
M3C2           ENTERED      -3.041886E-01      0.000000E+00
FECN_CHI       ENTERED      -3.826414E-01      0.000000E+00
M5C2           ENTERED      -5.420475E-01      0.000000E+00
ENTERED PHASES WITH DRIVING FORCE LESS THAN  -5.841299E-01
LIQUID SIGMA CHI A12 LAVES PHASE_C14 FE4N LP1 DIAMOND FCC_A4 KSI CARBIDE
FE8SI2C G PHASE M3SI NI3TI NBNI3 M5SI3 CR3SI MSI SIC AL4C3 GAS
*** STATUS FOR ALL SPECIES
C ENTERED      C4 ENTERED      CR ENTERED      NI ENTERED
C2 ENTERED      C5 ENTERED      FE ENTERED      SI ENTERED
C3 ENTERED      C60 ENTERED     MN ENTERED      VA ENTERED
POLY_3: @@ Now determine maximum temperature where no Ferrite (BCC_A2) exists

```

```

POLY_3: @@ Use
POLY_3: c-t
... the command in full is COMPUTE_TRANSITION
This command is a combination of CHANGE_STATUS and SET_CONDITION
to calculate directly when a phase may form by releasing one condition.
Phase to form: bcc_a2
You want to find when the current major phase is formed, please give
New major phase: fcc_a1
You must release one of these conditions
T=915.221, W(C)=5.5E-3, W(CR)=2.93768E-2, W(MN)=3E-3, W(NI)=2.8E-2,
W(SI)=3E-3, P=1E5, N=1 DEGREES OF FREEDOM 0
Give the state variable to be removed /T/: t
Testing POLY result by global minimization procedure
Calculated 23376 grid points in 1 s
To form BCC_A2 the condition is set to T=1012.45181314
POLY_3:
POLY_3: show tc
... the command in full is SHOW_VALUE
TC=739.45181
POLY_3:Hit RETURN to continue
POLY_3: @@ Check how this varies with the carbon content
POLY_3: ch-st phase fcc_a1
... the command in full is CHANGE_STATUS
Status: /ENTERED/: ent
Start value, number of moles /0/: 1
POLY_3: ch-st phase bcc_a2
... the command in full is CHANGE_STATUS
Status: /ENTERED/: fix
Number of moles /0/: 0
POLY_3:
POLY_3: s-c t=none
... the command in full is SET_CONDITION
POLY_3:
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 23376 grid points in 0 s
7 ITS, CPU TIME USED 0 SECONDS
POLY_3: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: TCFE7

Conditions:
W(C)=5.5E-3, W(CR)=2.93768E-2, W(MN)=3E-3, W(NI)=2.8E-2, W(SI)=3E-3, P=1E5,
N=1
FIXED PHASES
BCC_A2=0
DEGREES OF FREEDOM 0

Temperature 1012.45 K ( 739.30 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 5.45430E+01
Total Gibbs energy -4.54060E+04, Enthalpy 2.77487E+04, Volume 7.08402E-06

Component      Moles      W-Fraction  Activity   Potential  Ref.stat
C               2.4976E-02  5.5000E-03  7.8817E-02 -2.1387E+04 SER
CR              3.0816E-02  2.9377E-02  4.6417E-04 -6.4611E+04 SER
FE              9.0938E-01  9.3112E-01  5.7861E-03 -4.3372E+04 SER
MN              2.9784E-03  3.0000E-03  4.5168E-06 -1.0361E+05 SER
NI              2.6022E-02  2.8000E-02  8.0605E-05 -7.9348E+04 SER
SI              5.8260E-03  3.0000E-03  3.6734E-10 -1.8288E+05 SER

FCC_A1          Status ENTERED      Driving force 0.0000E+00
Moles 9.6176E-01, Mass 5.2968E+01, Volume fraction 9.6838E-01 Mass fractions:
FE 9.46531E-01 CR 1.55549E-02 C 3.06184E-03
NI 2.88106E-02 SI 3.08922E-03 MN 2.95285E-03

M7C3           Status ENTERED      Driving force 0.0000E+00
Moles 3.8245E-02, Mass 1.5752E+00, Volume fraction 3.1623E-02 Mass fractions:
CR 4.94158E-01 C 8.74860E-02 NI 7.42624E-04
FE 4.13028E-01 MN 4.58537E-03 SI 5.68368E-11

BCC_A2          Status FIXED      Driving force 0.0000E+00
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
FE 9.71740E-01 CR 1.04725E-02 MN 8.83251E-04
NI 1.30178E-02 SI 3.81249E-03 C 7.40352E-05
POLY_3: show tc
... the command in full is SHOW_VALUE
TC=739.45181
POLY_3:
POLY_3:Hit RETURN to continue
POLY_3:
POLY_3: s-a-v 1 w(c) 0 .08 0.001,,,
... the command in full is SET_AXIS_VARIABLE
POLY_3: save tcex07 y
... the command in full is SAVE_WORKSPACES
POLY_3: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 0.550000E-02
...OK

Phase Region from 0.550000E-02 for:
BCC_A2
FCC_A1
M7C3
Global check of adding phase at 8.31547E-03
Calculated 5 equilibria

Phase Region from 0.831547E-02 for:
BCC_A2
CEMENTITE
FCC_A1
M7C3
Global check of removing phase at 1.15396E-02
Calculated 7 equilibria

Phase Region from 0.115396E-01 for:
BCC_A2
CEMENTITE
FCC_A1
Global test at 1.95000E-02 .... OK
Global check of adding phase at 2.30282E-02
Calculated 14 equilibria

```

```

Phase Region from 0.230282E-01 for:
  BCC_A2
  CEMENTITE
  FCC_A1
  GRAPHITE
Global test at 3.05000E-02 .... OK
Global test at 4.05000E-02 .... OK
Global test at 5.05000E-02 .... OK
Global test at 6.05000E-02 .... OK
Global test at 7.05000E-02 .... OK
Global test at 8.00000E-02 .... OK
Terminating at 0.80000E-01
Calculated 61 equilibria

Phase Region from 0.550000E-02 for:
  BCC_A2
  FCC_A1
  M7C3
Global check of removing phase at 1.56897E-03
Calculated 6 equilibria

Phase Region from 0.156897E-02 for:
  BCC_A2
  FCC_A1
Global test at 1.00115E-15 .... OK
Terminating at 0.215894E-12
Calculated 5 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex07\tcex
07.POLY3
POLY_3: post

```

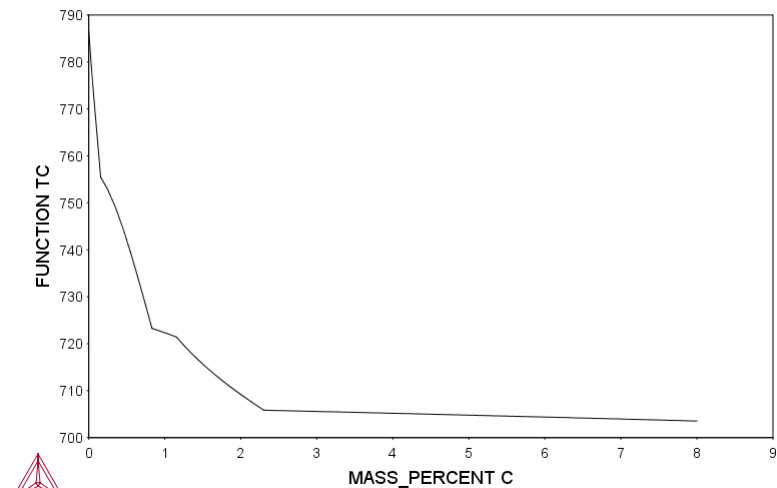
POLY-3 POSTPROCESSOR VERSION 3.2

```

POST: s-d-a x w-p c
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y tc
... the command in full is SET_DIAGRAM_AXIS
POST:
POST: set-title example 7a
POST: plot
... the command in full is PLOT DIAGRAM
                                example 7a

```

2016.05.16.13.12.48  
TCFE7: C, CR, FE, MN, NI, SI  
W(CR)=2.93768E-2, W(MN)=3E-3, W(NI)=2.8E-2, W(SI)=3E-3, P=1E5, N=1.



```

POST:
POST:Hit RETURN to continue
POST: s-s y n 700 800
... the command in full is SET_SCALING_STATUS
POST: s-lab b
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 7b
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

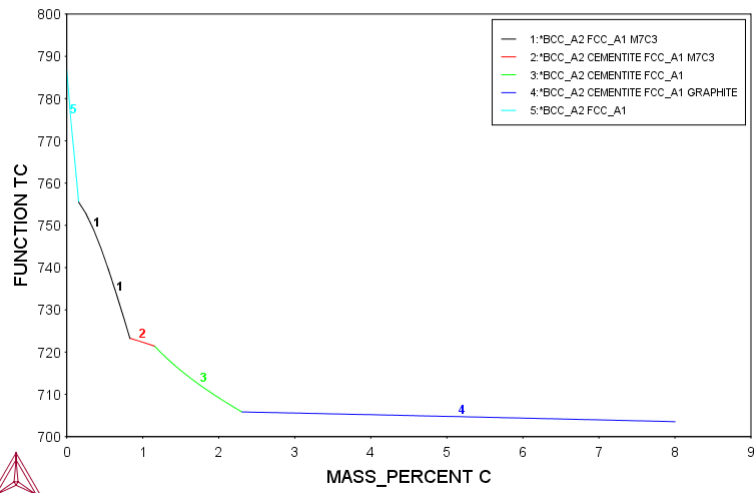
```

### example 7b

2016.05.16.13.12.49

TCFE7: C, CR, FE, MN, NI, SI

W(CR)=2.93768E-2, W(MN)=3E-3, W(NI)=2.8E-2, W(SI)=3E-3, P=1E5, N=1.



POST:

POST: set-inter

... the command in full is SET\_INTERACTIVE\_MODE

POST:

tcex08

## About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software (build 9533) running on WinNT 64-bit wordlength  
Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118  
License library version: 8.5.1.0017  
Linked: Mon May 16 09:31:44 2016

```
SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex08\tcex08.TCM" set-echo
```

```
SYS: @@
```

```
SYS: @@
```

```
SYS: @@ Calculation of a property diagram for a high speed steel
```

```
SYS: @@ i.e. phase fraction plots, activity vs temperature etc.
```

```
SYS: @@
```

```
SYS: set-log ex08,,
```

```
SYS: go p-3
```

```
... the command in full is GOTO_MODULE
```

```
POLY version 3.32
```

```
POLY_3: def-dia
```

```
... the command in full is DEFINE_DIAGRAM
```

```
For binary or ternary diagrams you may prefer the special modules
```

You must specify a value for all compositions and the temperature even  
if you want to use it as axis.

THERMODYNAMIC DATABASE module

Current database: Steels/Fe-Alloys v8.0

```
VA DEFINED
```

```
L12_FCC
```

```
B2_BCC
```

```
B2_VACANCY
```

```
HIGH_SIGMA
```

```
DICTRA_FCC_A1 REJECTED
```

```
Database /TCFE8/: tcfe7
```

Current database: Steels/Fe-Alloys v7.0

```
VA DEFINED
```

```
L12_FCC
```

```
B2_BCC
```

```
B2_VACANCY
```

```
HIGH_SIGMA
```

```
DICTRA_FCC_A1 REJECTED
```

```
Major element or alloy: fe
```

```
Composition input in mass (weight) percent? /Y/:
```

```
1st alloying element: c .9 cr 4 mn .3 si .3 w 8 mo 5 v 2
```

```
Next alloying element:
```

```
Temperature (C) /1000/: 1000
```

```
VA DEFINED
```

```
L12_FCC
```

```
B2_BCC
```

```
B2_VACANCY
```

```
HIGH_SIGMA
```

```
DICTRA_FCC_A1 REJECTED
```

```
REINITIATING GES5 .....
```

```
... the command in full is DEFINE_ELEMENTS
```

```
FE DEFINED
```

```
... the command in full is DEFINE_ELEMENTS
```

```
C DEFINED
```

```
... the command in full is DEFINE_ELEMENTS
```

```
CR DEFINED
```

```
... the command in full is DEFINE_ELEMENTS
```

```
MN DEFINED
```

```
... the command in full is DEFINE_ELEMENTS
```

```
SI DEFINED
```

```
... the command in full is DEFINE_ELEMENTS
```

```
W DEFINED
```

```
... the command in full is DEFINE_ELEMENTS
```

```
MO DEFINED
```

```
... the command in full is DEFINE_ELEMENTS
```

```
V DEFINED
```

This database has following phases for the defined system

GAS:G	LIQUID:L	BCC_A2
FCC_A1	HCP_A3	DIAMOND_FCC_A4
GRAPHITE	CEMENTITE	M23C6
M7C3	M6C	M5C2
M3C2	MC_ETA	MC_SHP
KSI_CARBIIDE	Al_KAPPA	KAPPA
Z_PHASE	FE4N_LP1	FECN_CHI
SIGMA	MU_PHASE	P_PHASE
R_PHASE	CHI_A12	LAVES_PHASE_C14
M3SI	G_PHASE	CR3SI
FE2SI	MSI	M5SI3
AL4C3	FE8SI2C	SIC

```
Reject phase(s) /NONE/: NONE
```

```
Restore phase(s) /NONE/: NONE
```

```
.....
```

The following phases are retained in this system:

GAS:G	LIQUID:L	BCC_A2
FCC_A1	HCP_A3	DIAMOND_FCC_A4
GRAPHITE	CEMENTITE	M23C6
M7C3	M6C	M5C2
M3C2	MC_ETA	MC_SHP
KSI_CARBIIDE	Al_KAPPA	KAPPA
Z_PHASE	FE4N_LP1	FECN_CHI
SIGMA	MU_PHASE	P_PHASE
R_PHASE	CHI_A12	LAVES_PHASE_C14
M3SI	G_PHASE	CR3SI
FE2SI	MSI	M5SI3
AL4C3	FE8SI2C	SIC

```
.....
```

```
OK? /Y/: Y
```

```
ELEMENTS .....
```

```
SPECIES .....
```

```
PHASES .....
```

```
... the command in full is AMEND_PHASE_DESCRIPTION
```

```
... the command in full is AMEND_PHASE_DESCRIPTION
```

... the command in full is AMEND\_PHASE\_DESCRIPTION  
... the command in full is AMEND\_PHASE\_DESCRIPTION  
... the command in full is AMEND\_PHASE\_DESCRIPTION  
PARAMETERS ...  
FUNCTIONS ....

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-OK-

**Should any phase have a miscibility gap check? /N/:** N

Using global minimization procedure  
 Calculated 31641 grid points in 0 s  
 Found the set of lowest grid points in 0 s  
 Calculated POLY solution 0 s, total time 0 s  
 You must now set an independent axis for your diagram  
 as one of the following conditions:  
 Condition 1 is temperature (Celsius)  
 Condition 2 is mass percent of C  
 Condition 3 is mass percent of CR  
 Condition 4 is mass percent of MN  
 Condition 5 is mass percent of SI  
 Condition 6 is mass percent of W  
 Condition 7 is mass percent of MO  
 Condition 8 is mass percent of V

**Give the number of the condition to vary /1/:** 1

**Minimum value (C) /800/:** 600

**Maximum value (C) /1800/:** 1600

The second axis can be another of the conditions above and you will then calculate a phase diagram.  
 Or you may want to plot how some other quantities depend on the selected condition and you will then calculate a "property" diagram.

In addition to the conditions above you may use these selected dependent quantities on the vertical axis:  
 Dependent 9 is mass fraction of all phases  
 Dependent 10 is composition of a phase  
 Dependent 11 is the fraction of a component in all phases  
 (In the post processor you may select many other quantities)

**Give the number of the quantity on second axis /9/:** 9 tcex08 y

No initial equilibrium, using default  
 Step will start from axis value 1273.15  
 ...OK

Phase Region from 1273.15 for:  
 FCC\_A1  
 FCC\_A1#2  
 M6C

Global test at 1.35315E+03 .... OK  
 Global test at 1.45315E+03 .... OK  
 Global check of removing phase at 1.51799E+03  
 Calculated 27 equilibria

Phase Region from 1517.99 for:  
 FCC\_A1  
 M6C

Global check of adding phase at 1.51950E+03  
 Calculated 3 equilibria

Phase Region from 1519.50 for:  
 LIQUID  
 FCC\_A1  
 M6C

Global check of adding phase at 1.57015E+03  
 Calculated 8 equilibria

Phase Region from 1570.15 for:  
 LIQUID  
 BCC\_A2  
 FCC\_A1  
 M6C

Global check of removing phase at 1.57689E+03  
 Calculated 4 equilibria

Phase Region from 1576.89 for:  
 LIQUID  
 BCC\_A2  
 FCC\_A1

Global check of removing phase at 1.60196E+03  
 Calculated 5 equilibria

Phase Region from 1601.96 for:  
 LIQUID  
 BCC\_A2

Global Test at 1.67315E+03 .... OK  
 Global check of removing phase at 1.69052E+03  
 Calculated 12 equilibria

Phase Region from 1690.52 for:  
 LIQUID

Global test at 1.76315E+03 .... OK  
 Global test at 1.86315E+03 .... OK  
 Terminating at 1873.15  
 Calculated 22 equilibria

Phase Region from 1273.15 for:  
 FCC\_A1  
 FCC\_A1#2  
 M6C

Global test at 1.19315E+03 .... OK  
 Global check of adding phase at 1.12656E+03

```

Calculated      17 equilibria

Phase Region from      1126.56      for:
  FCC_A1
  FCC_A1#2
  M23C6
  M6C
Global check of adding phase at      1.11294E+03
Calculated      5 equilibria

Phase Region from      1112.94      for:
  BCC_A2
  FCC_A1
  FCC_A1#2
  M23C6
  M6C
Global check of removing phase at      1.09588E+03
Calculated      4 equilibria

Phase Region from      1095.88      for:
  BCC_A2
  FCC_A1#2
  M23C6
  M6C
Global test at      1.02315E+03 .... OK
Global test at      9.23150E+02 .... OK
Terminating at      873.150
Calculated      26 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex08\tcex
08.POLY3

```

```

POSTPROCESSOR VERSION 3.2

```

```

Setting automatic diagram axes
... the command in full is REINITIATE_PLOT_SETTINGS

POSTPROCESSOR VERSION 3.2

```

```

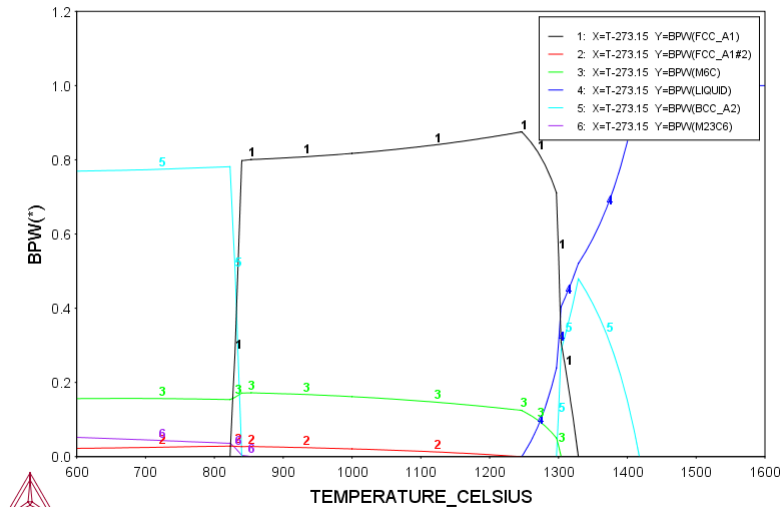
Setting automatic diagram axes
... the command in full is SET_AUTOMATIC_DIAGRAM_A

```

```

Setting automatic diagram axes
... the command in full is PLOT DIAGRAM
2016.05.16.13.15.22
TCFE7: C, CR, FE, MN, MO, SI, V, W
W(C)=9E-3, W(CR)=4E-2, W(MN)=3E-3, W(SI)=3E-3, W(W)=8E-2, W(MO)=5E-2, W(V)=2E-2, P=1E5, N=1.

```



```

POST:
POST:Hit RETURN to continue
POST: set-title example 8a
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

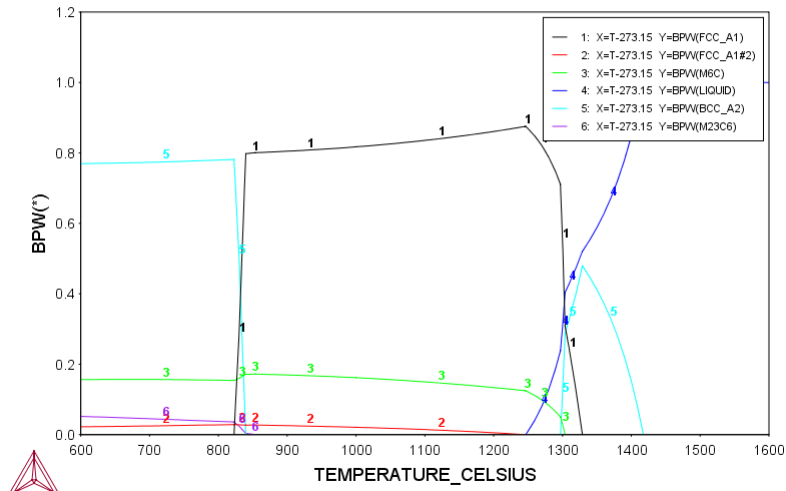
```

# example 8a

2016.05.16.13.15.24

TCFE7: C, CR, FE, MN, MO, SI, V, W

W(C)=9E-3, W(CR)=4E-2, W(MN)=3E-3, W(SI)=3E-3, W(W)=8E-2, W(MO)=5E-2, W(V)=2E-2, P=1E5, N=1.



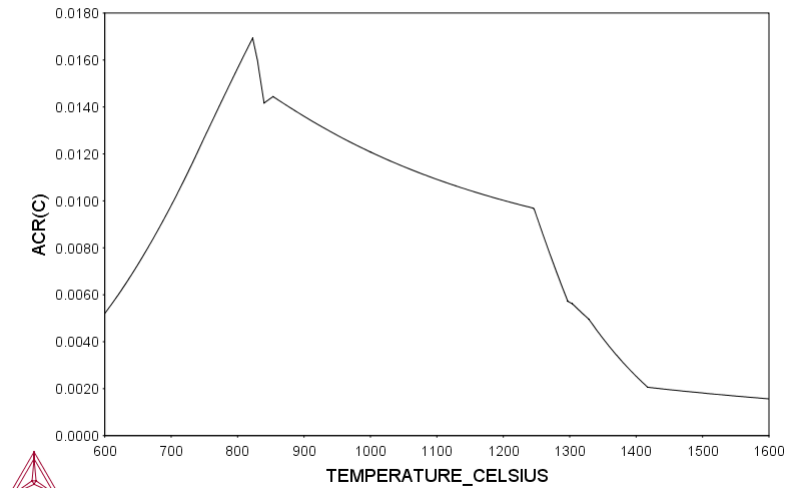
POST:  
 POST:Hit RETURN to continue  
 POST: s-d-a y acr(c)  
 ... the command in full is SET\_DIAGRAM\_AXIS  
 POST: set\_lab  
 ... the command in full is SET\_LABEL\_CURVE\_OPTION  
 CURVE LABEL OPTION (A, B, C, D, E, F OR N) /D/: n  
 POST: set-title example 8b  
 POST:  
 POST: plot  
 ... the command in full is PLOT DIAGRAM

## example 8b

2016.05.16.13.15.25

TCFE7: C, CR, FE, MN, MO, SI, V, W

W(C)=9E-3, W(CR)=4E-2, W(MN)=3E-3, W(SI)=3E-3, W(W)=8E-2, W(MO)=5E-2, W(V)=2E-2, P=1E5, N=1.



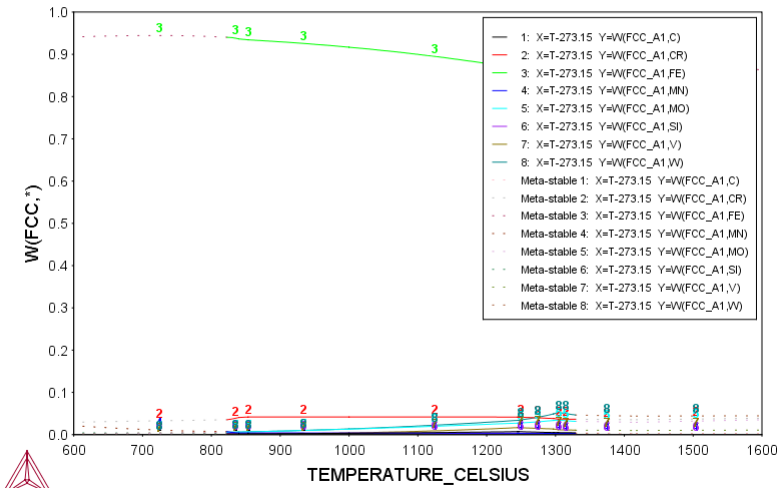
POST:  
 POST:Hit RETURN to continue  
 POST: @@ Plot how the composition of the austenite (called fcc) varies  
 POST: @@ Note this is plotted also where the austenite is not stable!  
 POST: s-d-a y w(fcc,\*)  
 ... the command in full is SET\_DIAGRAM\_AXIS  
 COLUMN NUMBER /\*/:  
 POST: set\_lab d  
 ... the command in full is SET\_LABEL\_CURVE\_OPTION  
 POST: set-title example 8c  
 POST:  
 POST: plot  
 ... the command in full is PLOT\_DIAGRAM

# example 8c

2016.05.16.13.15.27

TCFE7: C, CR, FE, MN, MO, SI, V, W

W(C)=9E-3, W(CR)=4E-2, W(MN)=3E-3, W(SI)=3E-3, W(W)=8E-2, W(MO)=5E-2, W(V)=2E-2, P=1E5, N=1.



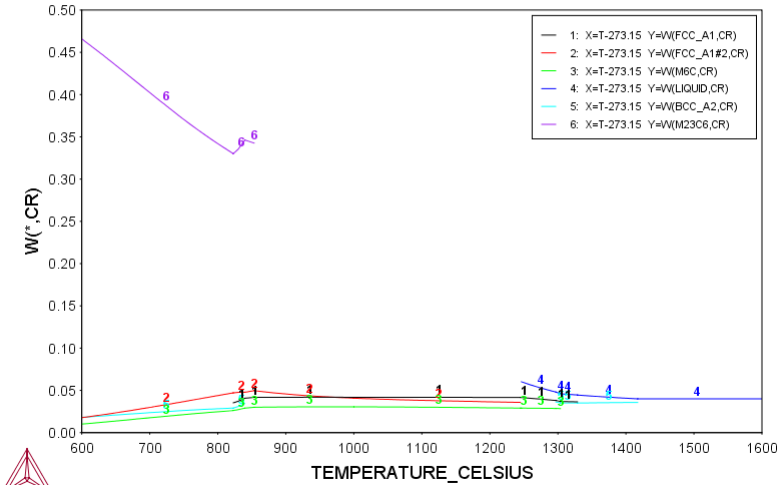
```
POST:
POST:Hit RETURN to continue
POST: @@ Plot the fraction of Cr in all phases
POST: s-d-a y w(*,cr)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: set-title example 8d
POST:
POST: plot
... the command in full is PLOT DIAGRAM
```

## example 8d

2016.05.16.13.15.29

TCFE7: C, CR, FE, MN, MO, SI, V, W

W(C)=9E-3, W(CR)=4E-2, W(MN)=3E-3, W(SI)=3E-3, W(W)=8E-2, W(MO)=5E-2, W(V)=2E-2, P=1E5, N=1.



```
POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex09

About

SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex09\tcex09.TCM" set-echo

SYS: @@

SYS: @@

SYS: @@ Calculation of dew point

SYS: @@

SYS:

SYS: go data

THERMODYNAMIC DATABASE module

Current database: Steels/Fe-Alloys v8.0

VA DEFINED

L12 FCC

B2 BCC

B2\_VACANCY

HIGH\_SIGMA

DICTRA\_FCC\_A1

REJECTED

TDB\_TCFE8: sw subdemo

Current database: Substance Demo Database

VA /- DEFINED

TDB\_SUBDEMO: def-sp h2 h2o1

H2 H2O1 DEFINED

TDB\_SUBDEMO: get

REINITIATING GES5 .....

ELEMENTS .....

SPECIES .....

PHASES .....

PARAMETERS ...

FUNCTIONS ....

List of references for assessed data

'H2<G> JANAF THERMOCHEMICAL TABLES SGTE \*\* H2<G> H2<G> HYDROGEN<G>

STANDARD STATE FROM CODATA KEY VALUES. CP FROM JANAF PUB. 3/61'

'H2O1<G> T.C.R.A.S. Class: 1 H2O1<G> H2O<G> WATER <GAS>, STEAM'

'H2O1<L> T.C.R.A.S. Class: 4 H2O1\_Liquid H2O\_Liquid Pure Water WATER

T.C.R.A.S. Class: 4 cp modified by atd 12/9/94 and 5/7/2002'

-OK-

TDB\_SUBDEMO: go p-3

POLY version 3.32

POLY\_3: s-c n=1 p=1e5 t=233

POLY\_3: ch-st ph h2o\_1=f 0

POLY\_3: c-e

Normal POLY minimization, not global

Testing POLY result by global minimization procedure

Calculated 138 grid points in 0 s

22 ITS, CPU TIME USED 0 SECONDS

POLY\_3: l-e,,,

Output from POLY-3, equilibrium = 1, label A0 , database: SUBDEMO

Conditions:

N=1, P=1E5, T=233

FIXED PHASES

H2O1\_L=0

DEGREES OF FREEDOM 0

Temperature 233.00 K ( -40.15 C), Pressure 1.000000E+05

Number of moles of components 1.00000E+00, Mass in grams 1.00931E+00

Total Gibbs energy -1.53589E+04, Enthalpy -9.53654E+02, Volume 9.68549E-03

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
-----------	-------	------------	----------	-----------	----------

H	9.9991E-01	9.9851E-01	3.6499E-04	-1.5335E+04	SER
---	------------	------------	------------	-------------	-----

O	9.3929E-05	1.4889E-03	1.0377E-61	-2.7203E+05	SER
---	------------	------------	------------	-------------	-----

GAS Status ENTERED Driving force 0.0000E+00

Moles 1.0000E+00, Mass 1.0093E+00, Volume fraction 1.0000E+00 Mass fractions:

H 9.9851E-01 O 1.4889E-03

Constitution:

H2 9.99812E-01 H2O1 1.87875E-04

H2O1\_L Status FIXED Driving force 0.0000E+00

Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:

O 8.88103E-01 H 1.11897E-01

POLY\_3: ent fun ph2\_h2o=acr(h2,gas)/acr(h2o,gas);

POLY\_3: s-a-v 1 t 173.15 373.15 ,

POLY\_3: save dew y

POLY\_3: step normal

No initial equilibrium, using default

Step will start from axis value 233.000

...OK

Phase Region from 233.000 for:

GAS

H2O1\_L

Global test at 2.73000E+02 .... OK

Global test at 3.23000E+02 .... OK

Global test at 3.73000E+02 .... OK

Terminating at 373.150

Calculated 32 equilibria

Phase Region from 233.000 for:

GAS

H2O1\_L

Global test at 1.93000E+02 .... OK

Terminating at 173.150

Calculated 15 equilibria

\*\*\* Buffer saved on file:

c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex09\dew.

POLY3

POLY\_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

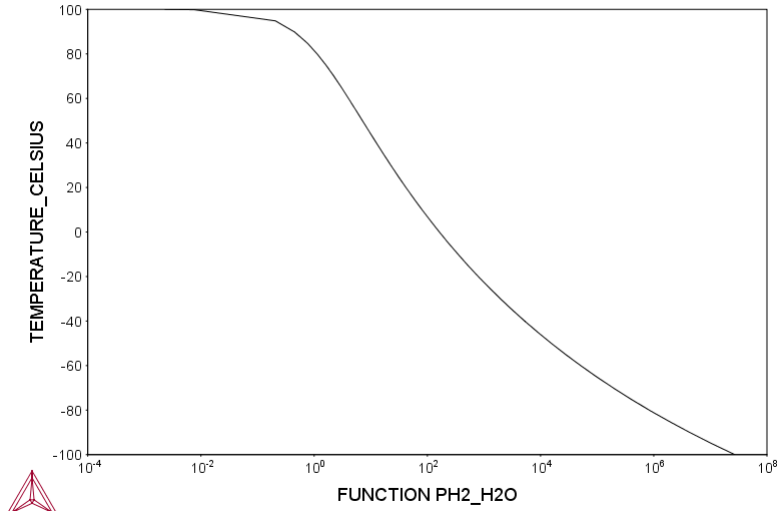
Setting automatic diagram axes

POST: s-d-a x ph2\_h2o

POST: s-a-ty x log

POST: s-d-a y t-c

POST: pl



POST:  
POST:  
POST: set-inter  
POST:

## About

```

SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex10\tcex10.TCM" set-echo
SYS: @@
SYS: @@ Preventing clogging of Cr2O3
SYS: @@ in a continuous casting process
SYS: @@
SYS: @@ Example showing how to avoid clogging
SYS: @@ in a continuous casting process
SYS: @@
SYS: @@ The background to this example is that a manufacturer wanted
SYS: @@ to increase the Cr content of a material from 18 to 25 weight
SYS: @@ percent. He then had trouble in the continous casting of this
SYS: @@ material because solid Cr2O3 was formed. By calculating the
SYS: @@ equilibria in the steel/slag system a simple correction could
SYS: @@ be found: modify the Mn or Si content, thus decrease the oxygen
SYS: @@ potential.
SYS: @@ In Thermo-calc, one can FIX a phase with zero amount to simulate
SYS: @@ how to avoid forming this phase. One should then release one of the
SYS: @@ conditions, usually one of the compositions, and this composition
SYS: @@ is determined by the equilibrium calculation.
SYS: @@
SYS: set-log ex10,,,,
SYS: @@ The user goes to the database module to obtain data
SYS: go da
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
L12_FCC B2_BCC B2_VACANCY
HIGH_SIGMA DICTRA_FCC_A1 REJECTED
TDB_TCFE8: @@ Switch to the database with slag data
TDB_TCFE8: sw slag3
... the command in full is SWITCH_DATABASE
Current database: Fe-containing Slag v3.2

FE O DEFINED
FEOLIQ REJECTED
TDB_SLAG3: @@ Some information about the database is given by this command
TDB_SLAG3: d-i
... the command in full is DATABASE_INFORMATION
Current database: Fe-containing Slag v3.2

SLAG3 -- TCS Fe-containing Slag Database
*****
(Version 3.2, August, 2012)

Copyright @ 1992-2012: Thermo-Calc Software, Stockholm, Sweden

This updated SLAG3 Slag Database contains a liquid SLAG phase, as well
as an Fe-rich liquid phase (dilute solution), a pure FeO liquid phase,
a large gaseous mixture phase (with neutral and charged inorganic, as
well as organic, gaseous species), and many stoichiometric solids and
solid solution phases (e.g., oxides, silicates, sulfides, halites,
etc.),
covering the following 30 elements:
Ag Al Ar B C Ca Co Cr Cu F
Fe H Mg Mn Mo N Na Nb Ni O
P Pb S Si Sn Ti U V W Zr
Thermodynamic data for the liquid SLAG phase and oxide/silicate solid
phases in the Al2O3-CaO-CrO-Cr2O3-FeO-Fe2O3-MgO-MnO-Na2O-SiO2-TiO2
system (with extensions to include sulfide/flouride and postulated
oxide/sulfide/flouride/silicate compounds) were critically assessed by
IRSID (1984) and TCS (since 1997), using the Kapoor-Frohberg-Gaye
Quasichemical Cell Model, i.e., the Kapoor-Frohberg Slag Model with the
extensions introduced by Gaye and Welfringer (1984) for complex
multicomponent liquid slag systems.
Data for the additional components S and F (as sulfide and fluoride
species in the framework of [Al+3, Ca+2, Cr+2, Cr+3, Fe+2, Fe+3, Mg+2,
Mn+2, Na+, Si+4, Ti+4, O-2, S-2 & F-] in the liquid SLAG phase and some
O-/S-/F-bearing solid slag phases, which were critically assessed by
IRSID (1997) and TCS (since 1997), have been added to the database,
and it thus allows calculations of sulfide capacities and many other
specific properties of liquid SLAG within the framework of 12 elements:
Al-Ca-Cr-Fe-Mg-Mn-Na-Si-Ti-O-S-F
More elements and in more redox-states will be gradually included in
future versions of the SLAG database.
Note that composition-dependent parameters in various solid solution
phases have not been considered yet in this particular SLAG3 version,
implying that at present all the solid phases are simply trated as
pure/stoichiometric phases. However, it has been planned at TCSAB to
include complex oxide/silicate/phosphate/sulfide/fluorite/... solid
solution phases in future versions of the SLAG database.
Data for a dilute solution of many elements in the Fe-rich liquid phase
FE_LIQUID are critically assessed and converted to regular solution
parameters according to Hillert (1986), with modified dilute solution
parameters (plus a quadratic term) in Fe-rich liquid from Sigworth
and Elliot (1974), so that it becomes a consistent thermodynamic model
and also generally improves the agreements of calculated results with
available experimental data obtained from steel-making metallurgical
processes. The following 26 dilute components are included in the
FE_LIQUID solution phase:
Ag Al B C Ca Co Cr Cu H Mg Mn Mo N Nb Ni O P Pb S Si Sn Ti U V W Zr
Thermodynamic data for the FE_LIQUID solution phase are evaluated at
infinite dilution and the recommended composition limit of any minority
component, in the 27-component diluted Fe-rich liquid, is only 0.1wt%.
In some cases, data could be used at much higher concentrations in the
Fe-rich liquid phase (i.e., liquid steel), but the user must carefully
check each of such cases.
The SLAG3 database is suitable and efficient for various equilibrium
calculations of activities, phase equilibria, phase diagrams and
many other properties in a wide range of metallurgical slag systems,
especially for (but not limited to) steel-making processes. It can
be used not only for slag system (liquid slag and solid slag phases)
but also for alloy-slag-gas heterogeneous interaction processes.
For steels and various alloys, as well as other substances or solution
phases, which are in interactions with the Fe-rich FE_LIQUID phase or
the liquid SLAG phase, thermodynamic data can be appended from other
available databases, such as TCFE, TCNI, SSOL+SSUB, SALT, TCMF, TCES,
TTAL/MG/NI/TI, TCAQ, AQS, GCE, NUMT, NUOX, etc. For more information

```

on such databases, please consult Thermo-Calc Software.

Release History:   Version 1.0 initial release,       1992  
                   Version 1.1 with minor improvements,   1998  
                   Version 2.0 with major improvements,   2002  
                   Version 2.1 with major improvements,   2003  
                   Version 2.2 with minor improvements,   2006  
                   Version 2.3 adding Ti-species/phases,   2006  
                   Version 2.4 with minor improvements,   2008  
                   Version 3.0 with major improvements,   2009  
                   Version 3.1 with major improvements,   2010  
                   Version 3.2 with minor improvements,   2012

Edited by: Pingfang Shi (Thermo-Calc Software, Sweden), 2002-2010.  
           Lina Kjellqvist (Thermo-Calc Software, Sweden), 2012.

**TDB\_SLAG3:Hit RETURN to continue**

**TDB\_SLAG3:** @@ The user defines his system by giving the elements. Note that Fe  
**TDB\_SLAG3:** @@ and O are included by default.

**TDB\_SLAG3:** d-sys mn si cr al  
     ... the command in full is DEFINE\_SYSTEM  
     MN                               SI                               CR  
     AL   DEFINED

**TDB\_SLAG3:** @@ 'GET' reads thermodynamic data from the database files to the  
**TDB\_SLAG3:** @@ program

**TDB\_SLAG3:** get  
     ... the command in full is GET\_DATA  
     REINITIATING GES5 .....  
     ELEMENTS .....  
     SPECIES .....  
     PHASES .....  
     ... the command in full is AMEND\_PHASE\_DESCRIPTION  
     ... the command in full is AMEND\_PHASE\_DESCRIPTION  
     ... the command in full is AMEND\_PHASE\_DESCRIPTION  
     PARAMETERS ...  
     FUNCTIONS ....

List of references for assessed data

'SLAG2 (2006): TCS Fe-Containing Slag Database, V2.3, owned and provided  
   by Thermo-Calc Software.'  
 'TCMP2 (2009): TCS Materials Processing Database, V2.5, owned and provided  
   by Thermo-Calc Software.'  
 'Pingfang Shi (2006), unpublished assessments of CrO/Cr2O3-bearing  
   systems. '  
 'Lina Kjellqvist (2012), unpublished assessments of Al2O3-SiO2 quasi  
   -binary system'  
 'L Kjellqvist (2005), unpublished assessments of TiO2-bearing quasi-binary  
   systems: Al2O3-TiO2, CaO-TiO2, MgO-TiO2, FeO-TiO2, Fe2O3-TiO2.'  
 'Pingfang Shi (2009), unpublished assessments of Fe3O4-bearing systems. '  
 'Pingfang Shi (2006), unpublished assessments of SiO2-bearing systems. '  
 -OK-

**TDB\_SLAG3:** go p-3  
     ... the command in full is GOTO\_MODULE

POLY version 3.32

**POLY\_3:** @@ There are many commands in the POLY-3 module  
**POLY\_3:** ?

    ... the command in full is HELP

ADD_INITIAL_EQUILIBRIUM	EXIT	REINITIATE_MODULE
ADVANCED_OPTIONS	GOTO_MODULE	SAVE_WORKSPACES
AMEND_STORED_EQUILIBRIA	HELP	SELECT_EQUILIBRIUM
BACK	INFORMATION	SET_ALL_START_VALUES
CHANGE_STATUS	LIST_AXIS_VARIABLE	SET_AXIS_VARIABLE
COMPUTE_EQUILIBRIUM	LIST_CONDITIONS	SET_CONDITION
COMPUTE_TRANSITION	LIST_EQUILIBRIUM	SET_INPUT_AMOUNTS
CREATE_NEW_EQUILIBRIUM	LIST_INITIAL_EQUILIBRIA	SET_INTERACTIVE
DEFINE_COMPONENTS	LIST_STATUS	SET_NUMERICAL_LIMITS
DEFINE_DIAGRAM	LIST_SYMBOLS	SET_REFERENCE_STATE
DEFINE_MATERIAL	LOAD_INITIAL_EQUILIBRIUM	SET_START_CONSTITUTION
DELETE_INITIAL_EQUILIB	MACRO_FILE_OPEN	SET_START_VALUE
DELETE_SYMBOL	MAP	SHOW_VALUE
ENTER_SYMBOL	POST	STEP_WITH_OPTIONS
EVALUATE_FUNCTIONS	READ_WORKSPACES	TABULATE

**POLY\_3:Hit RETURN to continue**

**POLY\_3:** @@ Some basic information is given by the INFORMATION command  
**POLY\_3:** @@ Look at example 1 for more details.

**POLY\_3:** info  
     ... the command in full is INFORMATION

**WHICH SUBJECT /PURPOSE/:** ?

WHICH SUBJECT

Specify a subject (or its abbreviation as long as it is unique, e.g.,  
 SIN, SIT, SOL, SPE, STATE, STEP, SYM, SYS, SUB, etc.) on which information  
 should be given, from the following subjects that are important to the use  
 of the POLY module:

PURPOSE	GETTING STARTED	USER INTERFACE
HELP	MACRO FACILITY	PRIVATE FILES
BASIC THERMODYNAMICS	SYSTEM AND PHASES	CONSTITUENTS AND SPECIES
SUBLATTICES	COMPONENTS	SITE AND MOLE FRACTIONS
COMPOSITION AND CONSTITUTION		CONCENTRATION
STATE VARIABLES	INTENSIVE VARIABLES	EXTENSIVE VARIABLES
DERIVED VARIABLES	UNITS	BASIC UNITS
SYSTEM UNITS	COMPONENT UNITS	PHASE UNITS
PHASE-COMPONENT UNITS	PHASE-SPECIES UNITS	USER-SPECIFIED UNITS
SYMBOLS	REFERENCE STATES	METASTABLE EQUILIBRIUM
CONDITIONS	AXIS-VARIABLES	SPECIAL OPTIONS
CALCULATIONS TYPES	SINGLE EQUILIBRIUM	INITIAL EQUILIBRIUM
STEPPING	SOLIDIFICATION PATH	PARAEQUILIBRIUM AND TO
MAPPING	PLOTTING OF DIAGRAMS	GLOBAL MINIMIZATION
DIAGRAM TYPES	BINARY DIAGRAMS	TERNARY DIAGRAMS
QUASI-BINARY DIAGRAMS	HIGHER ORDER DIAGRAMS	PROPERTY DIAGRAMS
POTENTIAL DIAGRAMS	POURBAIX DIAGRAMS	AQUEOUS SOLUTIONS
ORDER-DISORDER	TROUBLE SHOOTING	FAQ

If you are using the ED\_EXP module (the sub-module of the PARROT module),  
 you can also get detailed information of the following subject keywords  
 which are relevant to the EX\_EXP module:

EDEXP	for Edit-Experiment Module (ED-EXP)
EDPOLY	for Performance of POLY Commands in the ED_EXP Module
EDSPECIAL	for Special Commands only available in the ED_EXP Module
EDPOP	for Other Commands in the Experimental Data (POP or DOP) Files



## WHICH SUBJECT /PURPOSE/:

### PURPOSE

#### INTRODUCTION to the Equilibrium Calculation Module (POLY)

Knowledge of the thermodynamic equilibrium is an important factor for understanding properties of materials and processes. With a database of thermodynamic model parameters, it is possible to predict such properties and also to obtain driving forces for diffusion-controlled phase transformations and other dynamic processes.

With the comprehensive Equilibrium Calculation module, POLY ? it is possible to calculate many different kinds of equilibria and diagrams, in particular multicomponent phase diagrams. This is thus an important tool in developing new materials and processes. The current POLY module is its third version; this is why is often referred as POLY\_3 in the Thermo-Calc software.

Different kind of databases can be used with the POLY module, and thus it can be used for alloys or ceramic system, as well as gaseous equilibria, aqueous solution involved heterogeneous interaction systems. Since TCCN, up to 40 elements and 1000 species can be defined into a single system (previously 20 elements and 400 species) for equilibrium calculations.

Great care has been taken to provide the users with the most flexible tool. All normal thermodynamic state variables can be used to set as conditions in calculating equilibria, and as axes in plotting diagrams. A unique facility is to set the composition or any property of an individual phase as a condition. Any state variable can be varied along an axis in order to generate a diagram. During calculations of a diagram, complete descriptions of all calculated equilibria are stored, and in the diagram any state variable can be used as axis.

One of the major improvements since the TCCR/TCW4 software version is that the recently-implemented Global Minimization Technique is used to assure that the present minimum in an equilibrium calculation is the most stable minima for the specified conditions. This new technique, which is based on the traditional GEM (Gibbs Energy Minimization) Technique (i.e., the ordinary POLY Minimization routines used in previous versions, where pre-knowledge of miscibility gaps in involved phases are necessary, otherwise, metastable equilibria instead of the stable equilibria may be obtained), will ultimately prevent a calculation from reaching an undesired metastable or unstable (local) equilibrium in a defined system, and automatically detect possible miscibility gap(s) and automatically create additional composition sets in a solution phase if needed for handling single or multiple miscibility gaps. Therefore it is no longer necessary for the user to specify additional composition sets in advance.

A Direct Global Minimization can be performed on conditions: N, n(comp), B, b(comp), w(comp), x(comp), T, and P, but not when combined conditions as e.g.  $w(a)-3*w(b)=1$  are used or when an activity or potential condition is used. For all other types of conditions where regular minimization converges, Indirect Global Minimization, i.e. global test and corrections, if necessary, are performed until the lowest minimum is found.

- \* Direct Global Minimization: From the mesh of Gibbs energy, find the set of grid points that gives the lowest energy solution under the specified conditions. This set of grid points provides starting combination of phases and their constitutions for regular minimization to find the exact equilibrium solution. This solution will be then subject to a global test as described below.
- \* Indirect Global Minimization: Under certain conditions, direct approach is impossible. In this case, regular minimization is performed first and then a check is performed in order to see if the found local minimum is a global one by checking if all grid points are above the equilibrium Gibbs energy plane. If not, then recalculate by including these grid points until no grid point is above the equilibrium Gibbs energy plane from the previous step.

The full-scale and full-scope usage of the Global Minimization Technique has been extended from for only single-point calculations within TCCR/TCW4 to for all types of calculations (of single-points, property diagram stepping and phase diagram mapping) within TCCS/TCW5.

The use of Global Minimization Technique may increase the computation time, while it is not an issue at all, thanks for the rapid developments of computer hardware nowadays.

- \* The main cost in time comes from the calculation of Gibbs energy at each grid point generated by properly meshing the composition space for each entered phase. In a typical multicomponent system calculation, about 100MB of RAM memory is needed in storing the mesh of Gibbs energies.
- \* An additional (but much smaller) cost in time comes from finding the set of grid points in the above mesh that give the lowest energy solution. This solution is where POLY starts its ordinary minimization. When POLY has found an equilibrium, the equilibrium Gibbs energy surface is compared to the mesh to assure that no grid point is below the surface, i.e. a global minimization has been reached.

Global Minimization is now performed by default in single-point or stepping or mapping equilibrium calculations, but can of course be turned off (and on again by repeating the command-sequence of ADVANCED OPTIONS GLOBAL MINIMIZATION) by the user for specific purposes. This means that truly stable equilibrium should be guaranteed for single-points, stepping and mapping calculations.

- \* A completely new stepping and mapping procedure that ensures Global Minimization everywhere it is critical has been developed and been made available in TCCS/TCW5. These newly re-written STEP/MAP routines are very important for stepping/mapping calculations in multicomponent systems where there are complex miscibility gaps in some phases, and it does not require having any ??good?? guess of starting points. Therefore, TCCS/TCW5 can automatically handle complex solution phases with single or multiple miscibility gaps [for instance, a solution phase that is thermodynamically described as a single phase in a Thermo-Calc database, such as FCC, BCC or HCP phases, may be split into two or several composition-sets/phases that are presented in an equilibrium state as metallic phase(s), carbide(s), nitride(s), carbonitride(s), nitrocarbide(s), and so on], and can thus ensure the correct and complete phase diagrams and property diagrams in multicomponent systems, without bothering staring points.

Together with the PARROT module, the POLY module is also used for critical assessment of experimental data in order to develop thermodynamic databases. The POLY module uses the Gibbs Energy System (GES) for modeling and data

manipulations of the thermodynamic properties of each phase.

The following commands are available in the POLY module:

```
POLY_3:
ADD_INITIAL_EQUILIBRIUM  EXIT                REINITIATE_MODULE
ADVANCED_OPTIONS         GOTO_MODULE          SAVE_WORKSPACES
AMEND_STORED_EQUILIBRIA  HELP                SELECT_EQUILIBRIUM
BACK                    INFORMATION           SET_ALL_START_VALUES
CHANGE_STATUS            LIST_AXIS_VARIABLE  SET_AXIS_VARIABLE
COMPUTE_EQUILIBRIUM      LIST_CONDITIONS    SET_CONDITION
COMPUTE_TRANSITION       LIST_EQUILIBRIUM    SET_INPUT_AMOUNTS
CREATE_NEW_EQUILIBRIUM   LIST_INITIAL_EQUILIBRIA SET_INTERACTIVE
DEFINE_COMPONENTS        LIST_STATUS        SET_NUMERICAL_LIMITS
DEFINE_DIAGRAM           LIST_SYMBOLS       SET_REFERENCE_STATE
DEFINE_MATERIAL          LOAD_INITIAL_EQUILIBRIUM SET_START_CONSTITUTION
DELETE_INITIAL_EQUILIB   MACRO_FILE_OPEN    SET_START_VALUE
DELETE_SYMBOL            MAP                SHOW_VALUE
ENTER_SYMBOL             POST               STEP_WITH_OPTIONS
EVALUATE_FUNCTIONS       READ_WORKSPACES     TABULATE
POLY_3:
```

Note that, since TCCS, the SPECIAL\_OPTIONS and SET\_MINIMIZATION\_OPTIONS commands (the later one was introduced in the TCCR version) has been merged into the new ADVANCED\_OPTIONS command; and the RECOVER\_START\_VALUES command has been removed, due to that is not relevant to the POLY module anymore.

Revision History of the POLY-Module User's Guide:

```
=====
Mar 1991  First release
          (Edited by Bo Jansson and Bo Sundman)
Oct 1993  Second revised release (with version J)
          (Edited by Bo Jansson and Bo Sundman)
Oct 1996  Third revised release (with version L)
          (Edited by Bo Sundman)
Nov 1998  Fourth revised release (with version M)
          (Edited by Bo Sundman)
Jun 2000  Fifth revised and extended release
          (Edited by Pingfang Shi)
Nov 2002  Sixth revised and extended release
          (Edited by Pingfang Shi)
May 2006  Eighth revised and extended release
          (Edited by Pingfang Shi)
Apr 2008  Ninth revised and extended release
          (Edited by Pingfang Shi)
```

WHICH SUBJECT:

POLY\_3:Hit RETURN to continue

POLY\_3: @@ Now set the conditions i.e. the temperature, pressure and

POLY\_3: @@ composition. We are interested in the situation at the

POLY\_3: @@ outflow of steel

POLY\_3: s-c t=1800,p=101325,n=1

... the command in full is SET\_CONDITION

POLY\_3: @@ As conditions one can specify that the steel should have

POLY\_3: @@ 18 weight percent of Cr, 0.4 w/o Mn and 0.4 w/o Si

POLY\_3: @@ (Note that the overall amount of Cr and Mn is not specified).

POLY\_3: s-c w(mn)=.004,w(cr)=.18,w(si)=.004

... the command in full is SET\_CONDITION

POLY\_3: @@ The amount of Al is very small, assume 7 ppm

POLY\_3: s-c w(al)=7e-6

... the command in full is SET\_CONDITION

POLY\_3: @@ We will later assume that the oxygen potential is determined

POLY\_3: @@ by the equilibrium with liquid slag but initially we assume

POLY\_3: @@ there is 100 ppm O

POLY\_3: s-c w(o)=1e-4

... the command in full is SET\_CONDITION

POLY\_3: l-c

... the command in full is LIST\_CONDITIONS

T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.18, W(SI)=4E-3, W(AL)=7E-6,  
W(O)=1E-4

DEGREES OF FREEDOM 0

POLY\_3:Hit RETURN to continue

POLY\_3: @@ Let us check what phases we have

POLY\_3: l-st p

... the command in full is LIST\_STATUS

\*\*\* STATUS FOR ALL PHASES

PHASE	STATUS	DRIVING FORCE	MOLES
SIO2_TRIDYMIT	ENTERED	0.000000E+00	0.000000E+00
SIO2_QUARTZ	ENTERED	0.000000E+00	0.000000E+00
SIO2_CRISTOBALITE	ENTERED	0.000000E+00	0.000000E+00
SIO2_BETA_QUARTZ	ENTERED	0.000000E+00	0.000000E+00
MNO_SIO2	ENTERED	0.000000E+00	0.000000E+00
MNO_AL2O3	ENTERED	0.000000E+00	0.000000E+00
MNO	ENTERED	0.000000E+00	0.000000E+00
MN2O2_SIO2	ENTERED	0.000000E+00	0.000000E+00
FEO_AL2O3	ENTERED	0.000000E+00	0.000000E+00
FEO	ENTERED	0.000000E+00	0.000000E+00
FE3O4	ENTERED	0.000000E+00	0.000000E+00
FE2O3	ENTERED	0.000000E+00	0.000000E+00
FE2O2_SIO2	ENTERED	0.000000E+00	0.000000E+00
CR2O3	ENTERED	0.000000E+00	0.000000E+00
AL6O9_SIO2O4	ENTERED	0.000000E+00	0.000000E+00
AL2O3	ENTERED	0.000000E+00	0.000000E+00
SLAG	ENTERED	0.000000E+00	0.000000E+00
FE_LIQUID	ENTERED	0.000000E+00	0.000000E+00
GAS	ENTERED	0.000000E+00	0.000000E+00

POLY\_3: @@ We start by assuming all other phases except FE\_LIQUID are suspended

POLY\_3: ch-st p \*=sus

... the command in full is CHANGE\_STATUS

POLY\_3: ch-st p fe-l=ent 0

... the command in full is CHANGE\_STATUS

POLY\_3: l-c

... the command in full is LIST\_CONDITIONS

T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.18, W(SI)=4E-3, W(AL)=7E-6,  
W(O)=1E-4

DEGREES OF FREEDOM 0

POLY\_3:Hit RETURN to continue

POLY\_3: @@ The degree of freedoms is zero and we can make a calculation.

POLY\_3: c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Using global minimization procedure

Calculated 20 grid points in 0 s

Found the set of lowest grid points in 0 s

Calculated POLY solution 0 s, total time 0 s

```

POLY_3: @@ Now set the suspended phases as dormant
POLY_3: c-st p *s=d
... the command in full is CHANGE_STATUS
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 20 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY_3: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES

```

PHASE	STATUS	DRIVING FORCE	MOLES
FE_LIQUID	ENTERED	0.000000E+00	1.000000E+00
AL2O3	DORMANT	-4.467190E-03	
AL6O9_SiO4	DORMANT	-4.414257E-02	
SLAG	DORMANT	-1.124576E-01	
MNO_AL2O3	DORMANT	-1.635823E-01	
FEO_AL2O3	DORMANT	-3.788023E-01	
SiO2_CRISTOBALITE	DORMANT	-4.217466E-01	
SiO2_TRIDYMIT	DORMANT	-4.221446E-01	
SiO2_BETA_QUARTZ	DORMANT	-4.449541E-01	
SiO2_QUARTZ	DORMANT	-4.449674E-01	
CR2O3	DORMANT	-4.826177E-01	

```

DORMANT PHASES WITH DRIVING FORCE LESS THAN -5.733375E-01
MNO SiO2 MN2O2 SiO2 Fe2O2 SiO2 MNO FEO Fe3O4 Fe2O3 GAS
POLY_3:Hit RETURN to continue
POLY_3: @@ If the stable phases do not change in 12 iterations the program
POLY_3: @@ terminates even if the program has not calculated the correct
POLY_3: @@ driving forces for the metastable phases.
POLY_3: @@ You can change that and other things by the command SET-NUMERICAL-LIMITS
POLY_3: @@ We now use that to change the lowest value of a fraction variable.
POLY_3: s-n-l 500 1E-6 1E-12 n
... the command in full is SET_NUMERICAL_LIMITS
LIMITATIONS of the present version of Thermo-Calc
Max number of elements : 40
Max number of species :5000
Max number of sublattices in a phase : 10
Max number of constituents in a phase: : 200
Max number of constituents in an ideal phase :5000

POLY_3:Hit RETURN to continue
POLY_3: @@ Calculate once more
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Using already calculated grid
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY_3: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES

```

PHASE	STATUS	DRIVING FORCE	MOLES
FE_LIQUID	ENTERED	0.000000E+00	1.000000E+00
AL2O3	DORMANT	-4.467190E-03	
AL6O9_SiO4	DORMANT	-4.414257E-02	
SLAG	DORMANT	-1.124576E-01	
MNO_AL2O3	DORMANT	-1.635823E-01	
FEO_AL2O3	DORMANT	-3.788023E-01	
SiO2_CRISTOBALITE	DORMANT	-4.217466E-01	
SiO2_TRIDYMIT	DORMANT	-4.221446E-01	
SiO2_BETA_QUARTZ	DORMANT	-4.449541E-01	
SiO2_QUARTZ	DORMANT	-4.449674E-01	
CR2O3	DORMANT	-4.826177E-01	

```

DORMANT PHASES WITH DRIVING FORCE LESS THAN -5.733375E-01
MNO SiO2 MN2O2 SiO2 Fe2O2 SiO2 MNO FEO Fe3O4 Fe2O3 GAS
POLY_3:Hit RETURN to continue
POLY_3: @@ The driving forces are quite stable.
POLY_3: @@ Now set the slag phase stable and let the program
POLY_3: @@ adjust the amount of oxygen to make it stable
POLY_3: c-st p slag=fix 0
... the command in full is CHANGE_STATUS
POLY_3: s-c w(o)
... the command in full is SET_CONDITION
Value /1E-04/: none
POLY_3: l-c
... the command in full is LIST_CONDITIONS
T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.18, W(SI)=4E-3, W(AL)=7E-6
FIXED PHASES
SLAG=0
DEGREES OF FREEDOM 0
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 426 grid points in 0 s
53 ITS, CPU TIME USED 4 SECONDS
POLY_3: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium = 1, label A0 , database: SLAG3

Conditions:
T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.18, W(SI)=4E-3, W(AL)=7E-6
FIXED PHASES
SLAG=0
DEGREES OF FREEDOM 0

Temperature 1800.00 K ( 1526.85 C), Pressure 1.013250E+05
Number of moles of components 1.00000E+00, Mass in grams 5.48777E+01
Total Gibbs energy -1.12615E+05, Enthalpy 7.09998E+04, Volume 0.00000E+00

Component      Moles      W-Fraction Activity Potential Ref.stat
AL              1.4237E-05  7.0000E-06  2.0544E-10 -3.3383E+05 SER
CR              1.8998E-01  1.8000E-01  5.0820E-04 -1.1351E+05 SER
FE              7.9778E-01  8.1187E-01  6.2366E-04 -1.1045E+05 SER
MN              3.9956E-03  4.0000E-03  2.3985E-06 -1.9367E+05 SER
O               4.1841E-04  1.2198E-04  4.1414E-13 -4.2672E+05 SER
SI              7.8159E-03  4.0000E-03  4.4720E-08 -2.5327E+05 SER

FE_LIQUID      Status ENTERED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 5.4878E+01, Volume fraction 0.0000E+00 Mass fractions:
FE 8.11871E-01 SI 4.00000E-03 O 1.21983E-04
CR 1.80000E-01 MN 4.00000E-03 AL 7.00000E-06

```

```

SLAG                      Status FIXED          Driving force 0.0000E+00
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
O 4.10814E-01 MN 1.72313E-01 CR 3.42320E-02
AL 2.73762E-01 SI 8.14396E-02 FE 2.74396E-02

AL2O3                      Status DORMANT        Driving force 9.9821E-02
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
AL 5.29261E-01 SI 0.00000E+00 FE 0.00000E+00
O 4.70739E-01 MN 0.00000E+00 CR 0.00000E+00

AL6O9_SI2O4                Status DORMANT        Driving force 6.7904E-02
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
O 4.88176E-01 SI 1.31839E-01 FE 0.00000E+00
AL 3.79984E-01 MN 0.00000E+00 CR 0.00000E+00
POLY_3:Hit RETURN to continue
POLY_3: @@ List also the status of the phases.
POLY_3: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE      STATUS      DRIVING FORCE      MOLES
SLAG       FIXED       0.000000E+00      0.000000E+00
FE_LIQUID  ENTERED      0.000000E+00      1.000000E+00
AL2O3      DORMANT      9.982100E-02
AL6O9_SI2O4 DORMANT      6.790401E-02
MNO_AL2O3  DORMANT     -6.090788E-02
FEO_AL2O3  DORMANT     -2.760540E-01
SIO2_CRISTOBALITE DORMANT -2.903040E-01
SIO2_TRIDYMITE DORMANT -2.907021E-01
SIO2_BETA_QUARTZ DORMANT -3.135115E-01
SIO2_QUARTZ DORMANT -3.135249E-01
CR2O3      DORMANT     -3.641846E-01
MNO_SIO2   DORMANT     -4.550160E-01
MN2O2_SIO2 DORMANT     -5.626559E-01
FE2O2_SIO2 DORMANT     -1.244157E+00
DORMANT PHASES WITH DRIVING FORCE LESS THAN -1.355940E+00
MNO FEO FE3O4 FE2O3 GAS 2
POLY_3:Hit RETURN to continue
POLY_3: @@ Note that mullite and corundum are stable!
POLY_3: @@ The amount of Al is probably too high, set it
POLY_3: @@ to half of the initial value
POLY_3: s-c w(al)=3.5e-6
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Using already calculated grid
76 ITS, CPU TIME USED 4 SECONDS
POLY_3: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE      STATUS      DRIVING FORCE      MOLES
SLAG       FIXED       0.000000E+00      0.000000E+00
FE_LIQUID  ENTERED      0.000000E+00      1.000000E+00
AL6O9_SI2O4 DORMANT      3.462882E-03
AL2O3      DORMANT     -5.440445E-02
SIO2_CRISTOBALITE DORMANT -1.302843E-01
SIO2_TRIDYMITE DORMANT -1.306824E-01
MNO_AL2O3  DORMANT     -1.367590E-01
SIO2_BETA_QUARTZ DORMANT -1.534919E-01
SIO2_QUARTZ DORMANT -1.535052E-01
CR2O3      DORMANT     -2.199493E-01
MNO_SIO2   DORMANT     -3.109704E-01
FEO_AL2O3  DORMANT     -3.517851E-01
MN2O2_SIO2 DORMANT     -4.254562E-01
DORMANT PHASES WITH DRIVING FORCE LESS THAN -1.106717E+00
FE2O2_SIO2 MNO FEO FE3O4 FE2O3 GAS F
POLY_3: @@ The Al2O3 phases are now not stable.
POLY_3: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: SLAG3

Conditions:
T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.18, W(SI)=4E-3, W(AL)=3.5E-6
FIXED PHASES
SLAG=0
DEGREES OF FREEDOM 0

Temperature 1800.00 K ( 1526.85 C), Pressure 1.013250E+05
Number of moles of components 1.00000E+00, Mass in grams 5.48735E+01
Total Gibbs energy -1.12649E+05, Enthalpy 7.09791E+04, Volume 0.00000E+00

Component      Moles      W-Fraction Activity Potential Ref.stat
AL              7.1180E-06 3.5000E-06 9.7338E-11 -3.4501E+05 SER
CR              1.8996E-01 1.8000E-01 5.0779E-04 -1.1352E+05 SER
FE              7.9769E-01 8.1184E-01 6.2371E-04 -1.1045E+05 SER
MN              3.9953E-03 4.0000E-03 2.3967E-06 -1.9368E+05 SER
O              5.3132E-04 1.5491E-04 5.2696E-13 -4.2312E+05 SER
SI              7.8153E-03 4.0000E-03 4.4640E-08 -2.5330E+05 SER

FE_LIQUID      Status ENTERED          Driving force 0.0000E+00
Moles 1.0000E+00, Mass 5.4873E+01, Volume fraction 0.0000E+00 Mass fractions:
FE 8.11842E-01 MN 4.00000E-03 O 1.54912E-04
CR 1.80000E-01 SI 4.00000E-03 AL 3.50000E-06

SLAG                      Status FIXED          Driving force 0.0000E+00
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
O 3.96074E-01 AL 1.63086E-01 CR 4.06215E-02
MN 2.36807E-01 SI 1.36167E-01 FE 2.72458E-02

AL6O9_SI2O4                Status DORMANT        Driving force 3.4629E-03
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
O 4.88176E-01 SI 1.31839E-01 FE 0.00000E+00
AL 3.79984E-01 MN 0.00000E+00 CR 0.00000E+00
POLY_3:Hit RETURN to continue
POLY_3: @@ We assume that this describes the situation at 18 w/o Cr. Some
POLY_3: @@ liquid slag that later will form mainly SiO2-Al2O3-MnO is present.
POLY_3: @@ Now increase the Cr-content to 25 w/o
POLY_3: s-c w(cr)=.25
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure

```

```

Using already calculated grid
  71 ITS, CPU TIME USED  4 SECONDS
POLY_3: l-e,,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: SLAG3

Conditions:
T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.25, W(SI)=4E-3, W(AL)=3.5E-6
FIXED PHASES
SLAG=0
DEGREES OF FREEDOM 0

Temperature 1800.00 K ( 1526.85 C), Pressure 1.013250E+05
Number of moles of components 1.00000E+00, Mass in grams 5.45773E+01
Total Gibbs energy -1.12779E+05, Enthalpy 7.08202E+04, Volume 0.00000E+00

Component      Moles      W-Fraction  Activity   Potential  Ref.stat
AL              7.0796E-06  3.5000E-06  7.7978E-11 -3.4833E+05 SER
CR              2.6241E-01  2.5000E-01  6.9368E-04 -1.0886E+05 SER
FE              7.2484E-01  7.4171E-01  5.6880E-04 -1.1183E+05 SER
MN              3.9737E-03  4.0000E-03  2.5522E-06 -1.9274E+05 SER
O               9.9119E-04  2.9056E-04  5.4210E-13 -4.2269E+05 SER
SI              7.7732E-03  4.0000E-03  4.4207E-08 -2.5344E+05 SER

FE_LIQUID      Status ENTERED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 5.4577E+01, Volume fraction 0.0000E+00 Mass fractions:
FE 7.41706E-01 SI 4.00000E-03 O 2.90561E-04
CR 2.50000E-01 MN 4.00000E-03 AL 3.50000E-06

SLAG           Status FIXED      Driving force 0.0000E+00
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
O 3.85022E-01 SI 1.41920E-01 CR 5.93665E-02
MN 2.64912E-01 AL 1.25822E-01 FE 2.29577E-02
POLY_3:Hit RETURN to continue
POLY_3: @@ Now Cr2O3 would like to be stable. The simplest correction is to modify
POLY_3: @@ the composition of the steel in order to decrease the oxygen potential.
POLY_3: @@ For example the Mn or Si content could be changed.
POLY_3: @@ In order to determine which of these has the largest influence
POLY_3: @@ on the oxygen potential, calculate this by the partial derivative
POLY_3: @@ of the oxygen activity w.r.t. the Mn and Si content.
POLY_3: s-ref-s o gas
... the command in full is SET_REFERENCE_STATE
Temperature /*/:
Pressure /1E5/:
POLY_3: show acr(o)
... the command in full is SHOW_VALUE
ACR(O)=7.9408178E-7
POLY_3: show acr(o).w(mn)
... the command in full is SHOW_VALUE
ACR(O).W(MN)=-4.6033449E-5
POLY_3: show acr(o).w(si)
... the command in full is SHOW_VALUE
ACR(O).W(SI)=-5.2536001E-5
POLY_3:Hit RETURN to continue
POLY_3: @@ The value is largest for Si and thus the smallest change is necessary
POLY_3: @@ for that. Instead of modifying this content in steps one may
POLY_3: @@ specify that the Cr2O3 phase should be on its limit of stability, i.e.
POLY_3: @@ set it FIX with zero amount and calculate the change in composition.
POLY_3: c-s p cr2o3=fix 0
... the command in full is CHANGE_STATUS
POLY_3: l-c
... the command in full is LIST CONDITIONS
T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.25, W(SI)=4E-3, W(AL)=3.5E-6
FIXED PHASES
SLAG=0 CR2O3=0
DEGREES OF FREEDOM -1
POLY_3: s-c w(si)=none
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 427 grid points in 0 s
  75 ITS, CPU TIME USED  4 SECONDS
POLY_3: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium = 1, label A0 , database: SLAG3

Conditions:
T=1800, P=1.01325E5, N=1, W(MN)=4E-3, W(CR)=0.25, W(AL)=3.5E-6
FIXED PHASES
SLAG=0 CR2O3=0
DEGREES OF FREEDOM 0

Temperature 1800.00 K ( 1526.85 C), Pressure 1.013250E+05
Number of moles of components 1.00000E+00, Mass in grams 5.46679E+01
Total Gibbs energy -1.12301E+05, Enthalpy 7.11953E+04, Volume 0.00000E+00

Component      Moles      W-Fraction  Activity   Potential  Ref.stat
AL              7.0913E-06  3.5000E-06  7.3390E-11 -3.4924E+05 SER
CR              2.6285E-01  2.5000E-01  6.9469E-04 -1.0883E+05 SER
FE              7.2776E-01  7.4346E-01  5.7139E-04 -1.1176E+05 SER
MN              3.9803E-03  4.0000E-03  2.4897E-06 -1.9311E+05 SER
O               1.0707E-03  3.1335E-04  9.0372E-07 -2.0828E+05 GAS
SI              4.3351E-03  2.2271E-03  2.3558E-08 -2.6286E+05 SER

FE_LIQUID      Status ENTERED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 5.4668E+01, Volume fraction 0.0000E+00 Mass fractions:
FE 7.43456E-01 MN 4.00000E-03 O 3.13352E-04
CR 2.50000E-01 SI 2.22708E-03 AL 3.50000E-06

SLAG           Status FIXED      Driving force 0.0000E+00
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
O 3.71218E-01 AL 1.53107E-01 CR 9.41709E-02
MN 2.62012E-01 SI 9.43792E-02 FE 2.51128E-02

CR2O3          Status FIXED      Driving force 0.0000E+00
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
CR 6.84207E-01 AL 0.00000E+00 FE 0.00000E+00
O 3.15793E-01 MN 0.00000E+00 SI 0.00000E+00
POLY_3:Hit RETURN to continue
POLY_3: @@ We can read the new Si content from this list but also

```

```

POLY_3: @@ show the value of a variable directly
POLY_3: sh w(si)
... the command in full is SHOW_VALUE
W(SI)=2.2270814E-3
POLY_3: @@ We have to increase the Si content to 0.4 w/o to avoid
POLY_3: @@ forming Cr2O3. Calculate also how much the Mn content must be changed
POLY_3: s-c w(si)=.004
... the command in full is SET_CONDITION
POLY_3: s-c w(mn)=none
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Using already calculated grid
104 ITS, CPU TIME USED 6 SECONDS
POLY_3: sh w(mn)
... the command in full is SHOW_VALUE
W(MN)=1.9763402E-3
POLY_3: @@ Check with Si content equal to 0.3. It should be consistent with
POLY_3: @@ the plot below, i.e. Mn content decreases with increasing Si content.
POLY_3: s-c w(si)=.003
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Using already calculated grid
78 ITS, CPU TIME USED 5 SECONDS
POLY_3: sh w(mn)
... the command in full is SHOW_VALUE
W(MN)=3.0479009E-3
POLY_3: Hit RETURN to continue
POLY_3: @@ Plot how the Mn content varies when the Si content
POLY_3: @@ varies between 0.2 and 0.8 w/o.
POLY_3: s-a-v 1 w(si) 0.002 0.008 0.0004
... the command in full is SET_AXIS_VARIABLE
POLY_3: save tcex10 y
... the command in full is SAVE_WORKSPACES
POLY_3: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 0.300000E-02
...OK

```

```

Phase Region from 0.300000E-02 for:
FE_LIQUID
SLAG
CR2O3
QBSMER trying to find equilibrium at 4.5200000E-03
QBSMER: Second global calculation
Calculated 9 equilibria
Sorry cannot continue 1717 55 1 4.4400000E-03

Phase Region from 0.300000E-02 for:
FE_LIQUID
SLAG
CR2O3
Terminating at 0.200000E-02
Calculated 6 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex10\tced
10.POLY3
POLY_3: post

```

POLY-3 POSTPROCESSOR VERSION 3.2

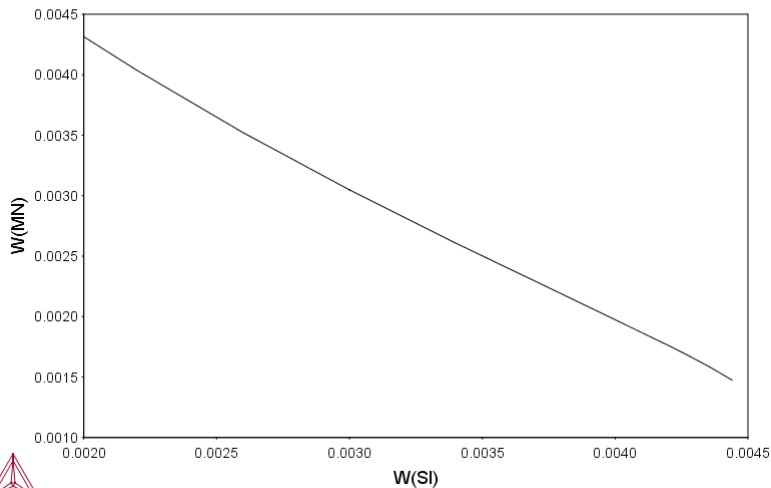
```

POST: s-d-a x w(si)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y w(mn)
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 10a
POST: plot
... the command in full is PLOT DIAGRAM

```

example 10a

2016.05.16.13.20.23  
SLAG3: AL, CR, FE, MN, O, SI  
T=1800, P=1.01325E5, N=1., W(CR)=0.25, W(AL)=3.5E-6



```

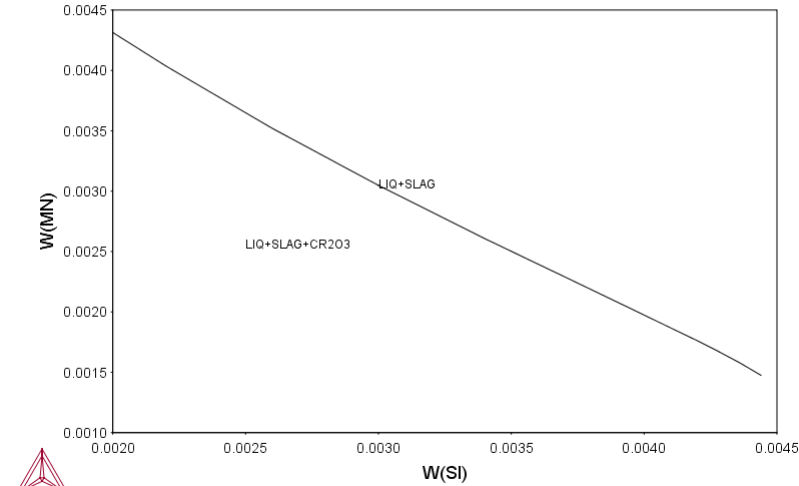
POST: Hit RETURN to continue
POST: add .003 .003 n
... the command in full is ADD_LABEL_TEXT
Text: LIQ+SLAG
Text size: /.36/
POST: add .0025 .0025 n
... the command in full is ADD_LABEL_TEXT

```

Text: LIQ+SLAG+CR2O3  
Text size: /.36/  
POST: set-title example 10b  
POST:  
POST: plot  
... the command in full is PLOT DIAGRAM

example 10b

2016.05.16.13.20.23  
SLAG3: AL, CR, FE, MN, O, SI  
T=1800, P=1.01325E5, N=1., W(CR)=0.25, W(AL)=3.5E-6



POST:  
POST: set-inter  
... the command in full is SET\_INTERACTIVE\_MODE  
POST:

tcex11

About License library version: 8.5.1.0017  
Linked: Mon May 16 09:31:44 2016

```
SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex11\tcex11.TCM" set-echo
SYS: @@
SYS: @@ Oxidation of Cu2S with H2O/O2 gas
SYS: @@
SYS: @@ Oxidation of Cu2S with H2O and O2 gas mixture
SYS: @@ Different O/H ratio represents different oxygen potential. Certain
SYS: @@ oxygen potential can desulphurize Cu2S without forming copper oxides.
SYS: @@ This example demonstrates how to find the optimum O/H ratio (i.e. oxygen
SYS: @@ potential).
SYS: @@ In Thermo-calc, the problem reduces to perform equilibria calculations in
SYS: @@ Cu-S-H-O system. The amounts of the components should be kept to correct
SYS: @@ ratio corresponding to Cu2S and H2O, by using a command SET_INPUT_
SYS: @@ AMOUNTS in POLY_3. Initially, O/H = 0.5 is given. Optimum O/H ratio
SYS: @@ is calculated by giving desired calculation conditions. For example,
SYS: @@ to simulate one phase disappearing, one can FIX the phase with zero amount
SYS: @@ in Thermo-calc.
SYS: @@
SYS: set-log ex11,,,
SYS: go da
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
L12 FCC B2_BCC B2_VACANCY
HIGH_SIGMA DICTRA_FCC_A1 REJECTED
TDB_TCFE8: sw
... the command in full is SWITCH_DATABASE
Use one of these databases

TCFE8 = Steels/Fe-Alloys v8.0
TCFE9 = Steels/Fe-Alloys v9.0 SNAPSHOT
FROST1 = FROST database v1.0
TCFE7 = Steels/Fe-Alloys v7.0
TCFE6 = Steels/Fe-Alloys v6.2
TCFE5 = Steels/Fe-Alloys v5.0
TCFE4 = Steels/Fe-Alloys v4.1
TCFE3 = Steels/Fe-Alloys v3.1
TCFE2 = Steels/Fe-Alloys v2.1
TCFE1 = Steels/Fe-Alloys v1.0
FEDAT = TCS/TT Steels Database v1.0
TCNI9 = Ni-Alloys v9.0 SNAPSHOT
TCNI8 = Ni-Alloys v8.0
TCNI7 = Ni-Alloys v7.1
TCNI6 = Ni-Alloys v6.0
TCNI5 = Ni-Alloys v5.1
TCNI4 = Ni-Alloys v4.0
TCNI1 = Ni-Alloys v1.3
TCAL4 = Al-Alloys v4.0
TCAL3 = Al-Alloys v3.0
TCAL2 = Al-Alloys v2.0
TCAL1 = Al-Alloys v1.2
TCMG5 = Mg-Alloys v5.0 SNAPSHOT
TCMG4 = Mg-Alloys v4.0
TCMG3 = Mg-Alloys v3.0
TCMG2 = Mg-Alloys v2.0
TCMG1 = Mg-Alloys v1.1
TCTI1 = Ti-Alloys v1.0 SNAPSHOT
TCCU1 = Copper v1.0 SNAPSHOT
TCCC1 = Cemented carbide v1.0
TCHEA1 = High Entropy Alloy v1.0
SSOL5 = SGTE Alloy Solutions Database v5.0
SSOL4 = SGTE Alloy Solutions Database v4.9f
SSOL2 = SGTE Alloy Solutions Database v2.1
SSUB5 = SGTE Substances Database v5.1
SSUB4 = SGTE Substances Database v4.1
SSUB3 = SGTE Substances Database v3.3
SSUB2 = SGTE Substances Database v2.2
SNOB3 = SGTE Nobel Metal Alloys Database v3.1
SNOB2 = SGTE Nobel Metal Alloys Database v2.1
SNOB1 = SGTE Nobel Metal Alloys Database v1.2
STBC2 = SGTE Thermal Barrier Coating TDB v2.2
STBC1 = SGTE Thermal Barrier Coating TDB v1.1
SALT1 = SGTE Molten Salts Database v1.2
SNUX6 = SGTE In-Vessel Nuclear Oxide TDB v6.2
SEMC2 = TC Semi-Conductors v2.1
SLAG4 = Fe-containing Slag v4.0 snapshot
SLAG3 = Fe-containing Slag v3.2
SLAG2 = Fe-containing Slag v2.2
SLAG1 = Fe-containing Slag v1.2
TCOX7 = Metal Oxide Solutions v7.0 SNAPSHOT
TCOX6 = Metal Oxide Solutions v6.1
TCOX5 = Metal Oxide Solutions v5.1
TCOX4 = Metal Oxide Solutions v4.1
ION3 = Ionic Solutions v3.0
ION2 = Ionic Solutions v2.6
ION1 = Ionic Solutions v1.5
NOX2 = NPL Oxide Solutions Database v2.1
TCSLD3 = Solder Alloys v3.1
TCSLD2 = Solder Alloys v2.0
TCSLD1 = Solder Alloys v1.0
TCSI1 = Ultrapure Silicon v1.1
TCMP2 = Materials Processing v2.5
TCES1 = Combustion/Sintering v1.1
TCSC1 = Super Conductor v1.0
TCFC1 = SOFC Database v1.0
TCNF2 = Nuclear Fuels v2.1b
NUMT2 = Nuclear Materials v2.1
NUOX4 = Nuclear Oxides v4.2
NUTO1 = U-Zr-Si Ternary Oxides TDB v1.1
NUTA1 = Ag-Cd-In Ternary Alloys TDB v1.1
NUCL10 = ThermoData NUCLEA Alloys-oxides TDB v10.2
MEPH11 = ThermoData MEPHISTA Nuclear Fuels TDB v11
TCAQ2 = Aqueous Solution v2.5
AQS2 = TGG Aqueous Solution Database v2.5
GCE2 = TGG Geochemical/Environmental TDB v2.3
PURE5 = SGTE Unary (Pure Elements) TDB v5.1
```



```

ALDEMO = Aluminum Demo Database
FEDEMO = Iron Demo Database
NIDEMO = Nickel Demo Database
SLDEMO = Solder Demo Database
OXDEMO = Oxide Demo Database
SUBDEMO = Substance Demo Database
PTERN = Public Ternary Alloys TDB v1.3
PAQ2 = Public Aqueous Soln (SIT) TDB v2.4
PG35 = G35 Binary Semi-Conductors TDB v1.2
MOB2 = Alloys Mobility v2.4
MOB1 = Alloys Mobility v1.3
MOBFE1 = Steels/Fe-Alloys Mobility v1.0
MOBFE2 = Steels/Fe-Alloys Mobility v2.0
MOBFE3 = Steels/Fe-Alloys Mobility v3.0
MOBNI4 = Ni-Alloys Mobility v4.0
MOBNI3 = Ni-Alloys Mobility v3.1
MOBNI2 = Ni-Alloys Mobility v2.4
MOBNI1 = Ni-Alloys Mobility v1.0
MOBAL3 = Al-Alloys Mobility v3.0
MOBAL2 = Al-Alloys Mobility v2.0
MOBAL1 = Al-Alloys Mobility v1.0
MOBCU1 = Cu-Alloys Mobility v1.0 SNAPSHOT
MOBMG1 = Mg-Alloys Mobility v1.0
MOBSI1 = Si-Alloys Mobility v1.0
MOBTI1 = Ti-Alloys Mobility v1.0
MALDEMO = Al-Alloys Mobility demo database
MFEDEMO = Fe-Alloys Mobility demo database
MNIDEMO = Ni-Alloys Mobility demo database
USER = User defined Database

```

```

DATABASE NAME /TCFE8/: user tcex11.tdb
Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

```

```

VA                /-  DEFINED
TDB_USER: def-sys cu s o h
... the command in full is DEFINE_SYSTEM
CU                S                O
H  DEFINED
TDB_USER: l-sys
... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:
GAS:G             :CU CU1H1 CU1H1O1 CU1O1 CU1S1 CU2 CU2S1 H H1O1 H1O1S1_HSO
H1O1S1_SOH H1O2 H1S1 H2 H2O1 H2O1S1_H2SO H2O1S1_HSOH H2O2 H2O4S1 H2S1 H2S2
O O1S1 O1S2 O2 O2S1 O3 O3S1 S S2 S3 S4 S5 S6 S7_S8:
CU                :CU:
CU2O              :CU2O1:
CU2O_L           :CU2O1:
CU2S             :CU2S1:
CU2S04           :CU2O4S1:
CU2S05           :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:
H2S04_L          :H2O4S1:
S                :S:
S_L              :S:
S_S2            :S:

```

```

TDB_USER:Hit RETURN to continue

```

```

TDB_USER: get
... the command in full is GET_DATA
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

```

```

List of references for assessed data

```

```

'TCS public data set for gaseous species, stoichiometric solids and
liquids in the Cu-Fe-H-N-O-S system.'

```

```

-OK-

```

```

TDB_USER: go p-3
... the command in full is GOTO_MODULE

```

```

POLY version 3.32

```

```

POLY_3: ?
... the command in full is HELP
ADD_INITIAL_EQUILIBRIUM EXIT REINITIATE_MODULE
ADVANCED_OPTIONS GOTO_MODULE SAVE_WORKSPACES
AMEND_STORED_EQUILIBRIA HELP SELECT_EQUILIBRIUM
BACK INFORMATION SET_ALL_START_VALUES
CHANGE_STATUS LIST_AXIS_VARIABLE SET_AXIS_VARIABLE
COMPUTE_EQUILIBRIUM LIST_CONDITIONS SET_CONDITION
COMPUTE_TRANSITION LIST_EQUILIBRIUM SET_INPUT_AMOUNTS
CREATE_NEW_EQUILIBRIUM LIST_INITIAL_EQUILIBRIA SET_INTERACTIVE
DEFINE_COMPONENTS LIST_STATUS SET_NUMERICAL_LIMITS
DEFINE_DIAGRAM LIST_SYMBOLS SET_REFERENCE_STATE
DEFINE_MATERIAL LOAD_INITIAL_EQUILIBRIUM SET_START_CONSTITUTION
DELETE_INITIAL_EQUILIB MACRO_FILE_OPEN SET_START_VALUE
DELETE_SYMBOL MAP SHOW_VALUE
ENTER_SYMBOL POST STEP_WITH_OPTIONS
EVALUATE_FUNCTIONS READ_WORKSPACES TABULATE

```

```

POLY_3: li-st
... the command in full is LIST_STATUS

```

```

Option /CPS/:

```

```

*** STATUS FOR ALL COMPONENTS
COMPONENT STATUS REF. STATE T(K) P(Pa)
VA ENTERED SER
CU ENTERED SER
H ENTERED SER
O ENTERED SER
S ENTERED SER
*** STATUS FOR ALL PHASES
PHASE STATUS DRIVING FORCE MOLES
S_S2 ENTERED 0.000000E+00 0.000000E+00
S_L ENTERED 0.000000E+00 0.000000E+00
S ENTERED 0.000000E+00 0.000000E+00
H2S04_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      0          ENTERED
CU1H1     ENTERED      H1O1      ENTERED      01S1     ENTERED
CU1H1009S1 ENTERED      H1O1S1_HSO ENTERED      01S2     ENTERED
CU1H101   ENTERED      H1O1S1_SOH ENTERED      02      ENTERED
CU1H2O2   ENTERED      H1O2      ENTERED      02S1     ENTERED
CU1H2O5S1 ENTERED      H1S1      ENTERED      03      ENTERED
CU1H607S1 ENTERED      H2        ENTERED      03S1     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
H1008S1   ENTERED      H8O7S1     ENTERED
POLY_3:
POLY_3:Hit RETURN to continue
POLY_3: @@ Assume initially that we have one mole of Cu2S and 50 moles water vapor
POLY_3: s-i-a n(cu2s1)=1,n(h2o1)=50
... the command in full is SET_INPUT_AMOUNTS
POLY_3: set-cond t=1400,p=101325
... the command in full is SET_CONDITION
POLY_3: l-c
... the command in full is LIST_CONDITIONS
N(CU)=2, N(S)=1, N(H)=100, N(O)=50, T=1400, P=1.01325E5
DEGREES OF FREEDOM 0
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      685 grid points in      0 s
Found the set of lowest grid points in      0 s
Calculated POLY solution      0 s, total time      0 s
POLY_3: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium =      1, label A0 , database: USER

Conditions:
N(CU)=2, N(S)=1, N(H)=100, N(O)=50, T=1400, P=1.01325E5
DEGREES OF FREEDOM 0

Temperature 1400.00 K ( 1126.85 C), Pressure 1.013250E+05
Number of moles of components 1.53000E+02, Mass in grams 1.05989E+03
Total Gibbs energy -2.75931E+07, Enthalpy -9.82382E+06, Volume 5.76972E+00

Component      Moles      W-Fraction Activity Potential Ref.stat
CU              2.0000E+00  1.1991E-01 1.6098E-03 -7.4867E+04 SER
H              1.0000E+02  9.5095E-02 9.5714E-06 -1.3452E+05 SER
O              5.0000E+01  7.5475E-01 5.1729E-11 -2.7570E+05 SER
S              1.0000E+00  3.0248E-02 2.0746E-08 -2.0593E+05 SER

GAS              Status ENTERED      Driving force 0.0000E+00
Moles 1.5022E+02, Mass 9.0794E+02, Volume fraction 1.0000E+00 Mass fractions:
O 8.81060E-01 H 1.11009E-01 S 7.92556E-03 CU 5.01241E-06
Constitution:
H2O1      9.86660E-01 CU1H1O1      1.96753E-08 CU1O1      8.58177E-12
H2        8.86811E-03 O3S1      1.43507E-08 H2O2      5.46461E-12
O2S1      4.44169E-03 H2O1S1_HSOH 7.52014E-09 H2O1S1_H2SO 3.12748E-12
H2S1      2.10471E-05 S        4.30477E-09 H2O4S1      3.10120E-12
O1S1      5.63051E-06 O2        2.46248E-09 S3        1.29650E-12
CU        1.32327E-06 H1O1S1_SOH 1.77241E-09 H1O2      4.13438E-13
H1O1      1.00104E-06 CU1S1      1.23642E-09 S4        3.25596E-18
H         4.55656E-07 CU2      4.47851E-10 S5        1.21560E-21
H1S1      3.40802E-07 CU2S1      2.11636E-10 O3        1.70006E-22
S2        1.38936E-07 H2S2      1.77731E-10 S6        5.54892E-27
CU1H1     8.04525E-08 O        4.66615E-11 S8        1.00000E-30
O1S2      2.49875E-08 H1O1S1_HSO 3.35706E-11 S7        1.00000E-30

CU2S_S3      Status ENTERED      Driving force 0.0000E+00
Moles 2.3266E+00, Mass 1.2343E+02, Volume fraction 0.0000E+00 Mass fractions:
CU 7.98557E-01 S 2.01443E-01 O 0.00000E+00 H 0.00000E+00

CU_L          Status ENTERED      Driving force 0.0000E+00
Moles 4.4883E-01, Mass 2.8522E+01, Volume fraction 0.0000E+00 Mass fractions:
CU 1.00000E+00 S 0.00000E+00 O 0.00000E+00 H 0.00000E+00
POLY_3:Hit RETURN to continue
POLY_3: @@ Now set the status of the diginite (CU2S_S3) to be fixed with
POLY_3: @@ zero amount. This means that we will reduce this completely
POLY_3: c-s
... the command in full is CHANGE_STATUS
For phases, species or components? /PHASES/:
Phase name(s): cu2s_s3
Status: /ENTERED/: fix
Number of moles /0/: 0
POLY_3: @@ We have now too many conditions as we must allow the gas to vary
POLY_3: @@ in composition to find the correct oxygen potential
POLY_3: l-c
... the command in full is LIST_CONDITIONS
N(CU)=2, N(S)=1, N(H)=100, N(O)=50, T=1400, P=1.01325E5
FIXED PHASES
CU2S_S3=0
DEGREES OF FREEDOM -1
POLY_3:Hit RETURN to continue
POLY_3: set-c n(o)=none
... the command in full is SET_CONDITION

```

```

POLY_3: l-c
... the command in full is LIST_CONDITIONS
N(CU)=2, N(S)=1, N(H)=100, T=1400, P=1.01325E5
FIXED PHASES
CU2S_S3=0
DEGREES OF FREEDOM 0
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 685 grid points in 0 s
10 ITS, CPU TIME USED 0 SECONDS
POLY_3: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium = 1, label A0 , database: USER

Conditions:
N(CU)=2, N(S)=1, N(H)=100, T=1400, P=1.01325E5
FIXED PHASES
CU2S_S3=0
DEGREES OF FREEDOM 0

Temperature 1400.00 K ( 1126.85 C), Pressure 1.013250E+05
Number of moles of components 1.54785E+02, Mass in grams 1.08845E+03
Total Gibbs energy -2.80759E+07, Enthalpy -1.00131E+07, Volume 5.85888E+00

Component      Moles      W-Fraction Activity Potential Ref.stat
CU              2.0000E+00  1.1676E-01  1.6098E-03 -7.4867E+04 SER
H              1.0000E+02  9.2600E-02  6.5700E-06 -1.3890E+05 SER
O              5.1785E+01  7.6118E-01  1.0863E-10 -2.6707E+05 SER
S              1.0000E+00  2.9455E-02  2.0746E-08 -2.0593E+05 SER

GAS              Status ENTERED      Driving force 0.0000E+00
Moles 1.5278E+02, Mass 9.6136E+02, Volume fraction 1.0000E+00 Mass fractions:
O 8.61805E-01 H 1.04841E-01 S 3.33486E-02 CU 4.75131E-06
Constitution:
H2O1 9.76211E-01 O1S2 5.24705E-08 H2O4S1 2.84109E-11
O2S1 1.95855E-02 CU1H1O1 2.83599E-08 CU1O1 1.80206E-11
H2 4.17844E-03 O2 1.08582E-08 H2O2 1.13535E-11
O1S1 1.18234E-05 H2O1S1_HSOH 7.44050E-09 H2O1S1_H2SO 3.09435E-12
H2S1 9.91688E-06 S 4.30477E-09 S3 1.29650E-12
H1O1 1.44290E-06 H1O1S1_SOH 2.55475E-09 H1O2 1.25138E-12
CU 1.32327E-06 CU1S1 1.23642E-09 S4 3.25596E-18
H 3.12773E-07 CU2 4.47851E-10 O3 1.57414E-21
H1S1 2.33934E-07 CU2S1 2.11636E-10 S5 1.21560E-21
S2 1.38936E-07 O 9.79832E-11 S6 5.54892E-27
O3S1 1.32878E-07 H2S2 8.37427E-11 S8 1.00000E-30
CU1H1 5.52244E-08 H1O1S1_HSO 4.83886E-11 S7 1.00000E-30

CU_L              Status ENTERED      Driving force 0.0000E+00
Moles 1.9999E+00, Mass 1.2709E+02, Volume fraction 0.0000E+00 Mass fractions:
CU 1.00000E+00 S 0.00000E+00 O 0.00000E+00 H 0.00000E+00

CU2S_S3              Status FIXED      Driving force 0.0000E+00
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
CU 7.98557E-01 S 2.01443E-01 O 0.00000E+00 H 0.00000E+00
POLY_3: sh n(*)
... the command in full is SHOW_VALUE
N(CU)=2, N(H)=100., N(O)=51.784749, N(S)=1.
POLY_3:Hit RETURN to continue
POLY_3: @@ If we have too much oxygen we may get some copper oxides,
POLY_3: @@ check which one is the closest to be stable
POLY_3: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE      STATUS      DRIVING FORCE      MOLES
CU2S_S3     FIXED      0.000000E+00      0.000000E+00
CU_L        ENTERED      0.000000E+00      1.999928E+00
GAS         ENTERED      0.000000E+00      1.527848E+02
CU2S_L      ENTERED      -3.931114E-04      0.000000E+00
CU2S_S2     ENTERED      -3.309936E-02      0.000000E+00
CU          ENTERED      -3.549960E-02      0.000000E+00
CU2S        ENTERED      -3.332974E-01      0.000000E+00
CU2O        ENTERED      -1.086153E+00      0.000000E+00
CU2O_L      ENTERED      -1.231036E+00      0.000000E+00
H2O_L       ENTERED      -1.738865E+00      0.000000E+00
CUS         ENTERED      -3.173417E+00      0.000000E+00
CUO         ENTERED      -3.229722E+00      0.000000E+00
CU2SO4      ENTERED      -3.322206E+00      0.000000E+00
ENTERED PHASES WITH DRIVING FORCE LESS THAN -3.797595E+00
CU2SO5 CUSO4 H2SO4_L H2O2_L S_L S2 S
POLY_3: @@ Set Cu2O to fix with zero amount and remove the fix status of CU2S_S3
POLY_3: c-s p cu2o=fix 0
... the command in full is CHANGE_STATUS
POLY_3: c-s p cu2s_s3
... the command in full is CHANGE_STATUS
Status: /ENTERED/:
Start value, number of moles /0/:
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 685 grid points in 0 s
39 ITS, CPU TIME USED 0 SECONDS
POLY_3: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: USER

Conditions:
N(CU)=2, N(S)=1, N(H)=100, T=1400, P=1.01325E5
FIXED PHASES
CU2O=0
DEGREES OF FREEDOM 0

Temperature 1400.00 K ( 1126.85 C), Pressure 1.013250E+05
Number of moles of components 1.54993E+02, Mass in grams 1.09178E+03
Total Gibbs energy -2.81294E+07, Enthalpy -1.00609E+07, Volume 5.85900E+00

Component      Moles      W-Fraction Activity Potential Ref.stat
CU              2.0000E+00  1.1641E-01  1.6098E-03 -7.4867E+04 SER
H              1.0000E+02  9.2317E-02  1.2909E-06 -1.5784E+05 SER
O              5.1993E+01  7.6191E-01  2.8253E-09 -2.2914E+05 SER
S              1.0000E+00  2.9365E-02  3.0696E-11 -2.8178E+05 SER

```

```

GAS                      Status ENTERED      Driving force 0.0000E+00
Moles 1.5299E+02, Mass 9.6469E+02, Volume fraction 1.0000E+00 Mass fractions:
O 8.6228E-01 H 1.0447E-01 S 3.3233E-02 CU 4.9735E-06
Constitution:
H2O1 9.8021E-01 H2O4S1 7.4267E-10 H1O1S1_HSO 3.6588E-13
O2S1 1.9603E-02 H2S1 5.6645E-10 CU2S1 3.1313E-13
H2 1.6131E-04 CU1O1 4.6870E-10 S2 3.0415E-13
H1O1 7.3737E-06 CU2 4.4785E-10 H2O1S1_H2SO 4.5971E-15
O2 7.3454E-06 H2O2 2.9650E-10 O3 2.7697E-17
O3S1 3.4592E-06 H1O2 1.6633E-10 H2S2 7.0774E-18
CU 1.3232E-06 H1S1 6.8008E-11 S3 4.1995E-21
O1S1 4.5500E-07 H1O1S1_SOH 1.9317E-11 S4 1.5604E-29
CU1H1O1 1.4493E-07 H2O1S1_HSOH 1.1054E-11 S7 1.0000E-30
H 6.1454E-08 S 6.3693E-12 S5 1.0000E-30
CU1H1 1.0850E-08 O1S2 2.9876E-12 S6 1.0000E-30
O 2.5484E-09 CU1S1 1.8293E-12 S8 1.0000E-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 1.0000E+00 S 0.0000E+00 O 0.0000E+00 H 0.0000E+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 8.8819E-01 O 1.1181E-01 S 0.0000E+00 H 0.0000E+00
POLY_3: show n(*)
... the command in full is SHOW VALUE
N(CU)=2, N(H)=100., N(O)=51.992866, N(S)=1.
POLY_3:Hit RETURN to continue
POLY_3: @@ The ratio N(O) to N(H) should thus be between 0.5178 and 0.52
POLY_3: @@ in order to reduce all Cu2S and not forming any Cu2O
POLY_3: @@ Make a diagram showing this amounts of phases
POLY_3: c-st p cu2o
... the command in full is CHANGE_STATUS
Status: /ENTERED/:
Start value, number of moles /0/:
POLY_3: s-a-v 1 n(o)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 45
Max value /1/: 55
Increment /.25/:
POLY_3: s-c n(o)
... the command in full is SET_CONDITION
Value /51.99286556/:
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 685 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY_3: save tcex11 y
... the command in full is SAVE_WORKSPACES
POLY_3: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 51.9929
...OK

Phase Region from 51.9929 for:
GAS
CU_L
Global check of adding phase at 5.19929E+01
Calculated 2 equilibria

Phase Region from 51.9929 for:
GAS
CU2O
CU_L
Global check of removing phase at 5.29928E+01
Calculated 6 equilibria

Phase Region from 52.9928 for:
GAS
CU2O
Global test at 5.49929E+01 .... OK
Terminating at 55.0000
Calculated 12 equilibria

Phase Region from 51.9929 for:
GAS
CU_L
Global check of adding phase at 5.17847E+01
Calculated 3 equilibria

Phase Region from 51.7847 for:
GAS
CU2S_S3
CU_L
Global test at 4.99929E+01 .... OK
Global test at 4.74929E+01 .... OK
Global test at 4.50000E+01 .... OK
Terminating at 45.0000
Calculated 31 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex11\tcex
11.POLY3
POLY_3: post

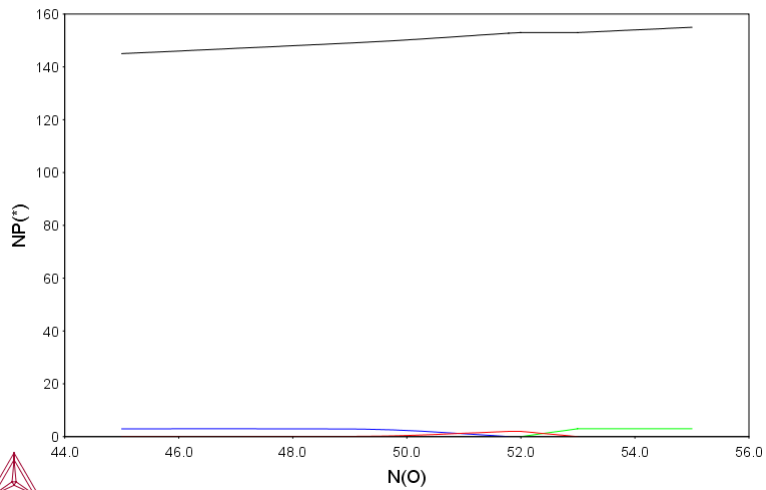
POLY-3 POSTPROCESSOR VERSION 3.2

POST: s-d-a x n(o)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y np(*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: set-title example 11a
POST: plot
... the command in full is PLOT_DIAGRAM

```

### example 11a

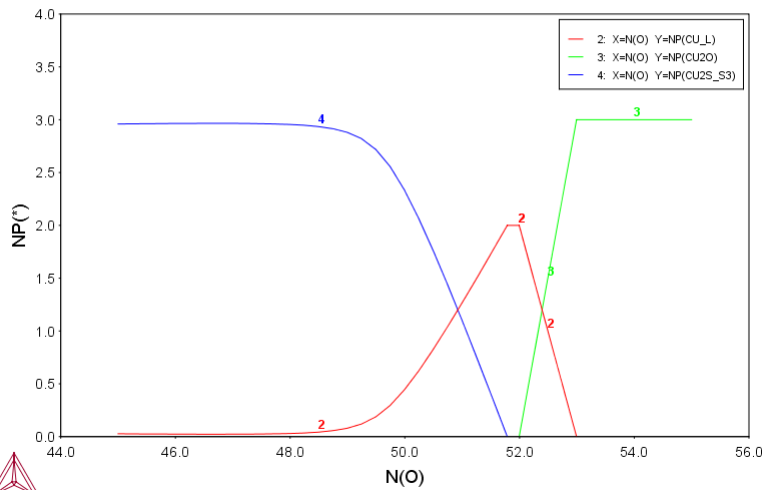
2016.05.16.13.22.34  
 USER: CU, H, O, S  
 N(CU)=2., N(S)=1., N(H)=100., T=1400, P=1.01325E5



POST:  
 POST:Hit RETURN to continue  
 POST: s-lab d  
 ... the command in full is SET\_LABEL\_CURVE\_OPTION  
 POST: s-s y n 0 4  
 ... the command in full is SET\_SCALING\_STATUS  
 POST: set-title example 11b  
 POST:  
 POST: plot  
 ... the command in full is PLOT DIAGRAM

### example 11b

2016.05.16.13.22.34  
 USER: CU, H, O, S  
 N(CU)=2., N(S)=1., N(H)=100., T=1400, P=1.01325E5



POST:  
 POST: set-inter  
 ... the command in full is SET\_INTERACTIVE\_MODE  
 POST:

## tcex12

**About** Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software (build 9533) running on WinNT 64-bit wordlength  
Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118  
License library version: 8.5.1.0017  
Linked: Mon May 16 09:31:44 2016

```
SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex12\tcex12.TCM" set-echo
```

```
SYS: @@  
SYS: @@ Tabulation  
SYS: @@ of thermodynamic data for reactions  
SYS: @@  
SYS: @@ This example shows a number of independent cases using the  
SYS: @@ tabulation module. This module is very rudimentary but still  
SYS: @@ provides some facilities. Note that there is no on-line help available!  
SYS: @@  
SYS: @@ Each case is separated by a line of =====  
SYS: set-log ex12,,  
SYS: go tab
```

```
... the command in full is GOTO_MODULE
```

```
TAB: ?
```

```
... the command in full is HELP
```

BACK	LIST_SUBSTANCES	SWITCH_DATABASE
ENTER_FUNCTION	MACRO_FILE_OPEN	TABULATE_DERIVATIVES
ENTER_REACTION	PATCH	TABULATE_REACTION
EXIT	SET_ENERGY_UNIT	TABULATE_SUBSTANCE
GOTO_MODULE	SET_INTERACTIVE	
HELP	SET_PLOT_FORMAT	

```
TAB: @@ Tabulate data for a reaction
```

```
TAB: tab-rea 3H2+N2=2N1H3;
```

```
... the command in full is TABULATE_REACTION
```

```
Use one of these databases
```

TCFE8	=	Steels/Fe-Alloys	v8.0
TCFE9	=	Steels/Fe-Alloys	v9.0 SNAPSHOT
FROST1	=	FROST database	v1.0
TCFE7	=	Steels/Fe-Alloys	v7.0
TCFE6	=	Steels/Fe-Alloys	v6.2
TCFE5	=	Steels/Fe-Alloys	v5.0
TCFE4	=	Steels/Fe-Alloys	v4.1
TCFE3	=	Steels/Fe-Alloys	v3.1
TCFE2	=	Steels/Fe-Alloys	v2.1
TCFE1	=	Steels/Fe-Alloys	v1.0
FEDAT	=	TCS/TT Steels Database	v1.0
TCNI9	=	Ni-Alloys	v9.0 SNAPSHOT
TCNI8	=	Ni-Alloys	v8.0
TCNI7	=	Ni-Alloys	v7.1
TCNI6	=	Ni-Alloys	v6.0
TCNI5	=	Ni-Alloys	v5.1
TCNI4	=	Ni-Alloys	v4.0
TCNI1	=	Ni-Alloys	v1.3
TCAL4	=	Al-Alloys	v4.0
TCAL3	=	Al-Alloys	v3.0
TCAL2	=	Al-Alloys	v2.0
TCAL1	=	Al-Alloys	v1.2
TCMG5	=	Mg-Alloys	v5.0 SNAPSHOT
TCMG4	=	Mg-Alloys	v4.0
TCMG3	=	Mg-Alloys	v3.0
TCMG2	=	Mg-Alloys	v2.0
TCMG1	=	Mg-Alloys	v1.1
TCTI1	=	Ti-Alloys	v1.0 SNAPSHOT
TCCU1	=	Copper	v1.0 SNAPSHOT
TCCC1	=	Cemented carbide	v1.0
TCHEA1	=	High Entropy Alloy	v1.0
SSOL5	=	SGTE Alloy Solutions Database	v5.0
SSOL4	=	SGTE Alloy Solutions Database	v4.9f
SSOL2	=	SGTE Alloy Solutions Database	v2.1
SSUB5	=	SGTE Substances Database	v5.1
SSUB4	=	SGTE Substances Database	v4.1
SSUB3	=	SGTE Substances Database	v3.3
SSUB2	=	SGTE Substances Database	v2.2
SNOB3	=	SGTE Nobel Metal Alloys Database	v3.1
SNOB2	=	SGTE Nobel Metal Alloys Database	v2.1
SNOB1	=	SGTE Nobel Metal Alloys Database	v1.2
STBC2	=	SGTE Thermal Barrier Coating TDB	v2.2
STBC1	=	SGTE Thermal Barrier Coating TDB	v1.1
SALT1	=	SGTE Molten Salts Database	v1.2
SNUX6	=	SGTE In-Vessel Nuclear Oxide TDB	v6.2
SEMC2	=	TC Semi-Conductors	v2.1
SLAG4	=	Fe-containing Slag	v4.0 snapshot
SLAG3	=	Fe-containing Slag	v3.2
SLAG2	=	Fe-containing Slag	v2.2
SLAG1	=	Fe-containing Slag	v1.2
TCOX7	=	Metal Oxide Solutions	v7.0 SNAPSHOT
TCOX6	=	Metal Oxide Solutions	v6.1
TCOX5	=	Metal Oxide Solutions	v5.1
TCOX4	=	Metal Oxide Solutions	v4.1
ION3	=	Ionic Solutions	v3.0
ION2	=	Ionic Solutions	v2.6
ION1	=	Ionic Solutions	v1.5
NOX2	=	NPL Oxide Solutions Database	v2.1
TCSLD3	=	Solder Alloys	v3.1
TCSLD2	=	Solder Alloys	v2.0
TCSLD1	=	Solder Alloys	v1.0
TCSI1	=	Ultrapure Silicon	v1.1
TCMP2	=	Materials Processing	v2.5
TCEs1	=	Combustion/Sintering	v1.1
TCSC1	=	Super Conductor	v1.0
TCFC1	=	SOFC Database	v1.0
TCNF2	=	Nuclear Fuels	v2.1b
NUMT2	=	Nuclear Materials	v2.1
NUOX4	=	Nuclear Oxides	v4.2
NUTO1	=	U-Zr-Si Ternary Oxides TDB	v1.1
NUTA1	=	Ag-Cd-In Ternary Alloys TDB	v1.1
NUCL10	=	ThermoData NUCLEA Alloys-oxides TDB	v10.2
MEPH11	=	ThermoData MEPHISTA Nuclear Fuels TDB	v11
TCAQ2	=	Aqueous Solution	v2.5
AQS2	=	TGG Aqueous Solution Database	v2.5
GCE2	=	TGG Geochemical/Environmental TDB	v2.3
PURE5	=	SGTE Unary (Pure Elements) TDB	v5.1

```

ALDEMO = Aluminum Demo Database
FEDEMO = Iron Demo Database
NIDEMO = Nickel Demo Database
SLDEMO = Solder Demo Database
OXDEMO = Oxide Demo Database
SUBDEMO = Substance Demo Database
PTERN = Public Ternary Alloys TDB v1.3
PAQ2 = Public Aqueous Soln (SIT) TDB v2.4
PG35 = G35 Binary Semi-Conductors TDB v1.2
MOB2 = Alloys Mobility v2.4
MOB1 = Alloys Mobility v1.3
MOBFE1 = Steels/Fe-Alloys Mobility v1.0
MOBFE2 = Steels/Fe-Alloys Mobility v2.0
MOBFE3 = Steels/Fe-Alloys Mobility v3.0
MOBNI4 = Ni-Alloys Mobility v4.0
MOBNI3 = Ni-Alloys Mobility v3.1
MOBNI2 = Ni-Alloys Mobility v2.4
MOBNI1 = Ni-Alloys Mobility v1.0
MOBAL3 = Al-Alloys Mobility v3.0
MOBAL2 = Al-Alloys Mobility v2.0
MOBAL1 = Al-Alloys Mobility v1.0
MOBCU1 = Cu-Alloys Mobility v1.0 SNAPSHOT
MOBMG1 = Mg-Alloys Mobility v1.0
MOBSI1 = Si-Alloys Mobility v1.0
MOBTI1 = Ti-Alloys Mobility v1.0
MALDEMO = Al-Alloys Mobility demo database
MFEDEMO = Fe-Alloys Mobility demo database
MNIDEMO = Ni-Alloys Mobility demo database
USER = User defined Database

```

```

DATABASE NAME /TCFE8/: SSUB5
THERMODYNAMIC DATABASE module
Current database: SGTE Substances Database v5.1

```

```

VA DEFINED
... the command in full is REJECT
VA DEFINED
REINITIATING GES5 .....
... the command in full is DEFINE_SPECIES
H2          N2          H3N1
  DEFINED
... the command in full is GET_DATA
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

```

List of references for assessed data

```

H2<G> JANAF THERMOCHEMICAL TABLES SGTE **
H2<G> H2<G>
HYDROGEN<G>
STANDARD STATE FROM CODATA KEY VALUES. CP FROM JANAF PUB. 3/61
H3N1<G> T.C.R.A.S. Class: 2
H3N1<G> NH3<G>
AMMONIA <GAS>
N2<G> JANAF THERMOCHEMICAL TABLES SGTE **
N2<G> N2<G>
NITROGEN <DIATOMIC GAS>
PUBLISHED BY JANAF AT 09/65

```

-OK-

```

Pressure /100000/: 100000
Low temperature limit /298.15/: 298.15
High temperature limit /2000/: 2000
Step in temperature /100/: 100

```

Output file /SCREEN/:

```

      O U T P U T   F R O M   T H E R M O - C A L C
      2016. 5.16                               13.24.37

```

```

Reaction:  3H2<G>+N2<G>=2H3N1<G>
H2<GAS>
N2<GAS>
H3N1<GAS>

```

```

*****
      T      Delta-Cp      Delta-H      Delta-S      Delta-G
      (K)      (Joule/K)      (Joule)      (Joule/K)      (Joule)
*****
298.15  -4.44006E+01  -9.18800E+04  -1.98115E+02  -3.28120E+04
300.00  -4.43267E+01  -9.19621E+04  -1.98389E+02  -3.24452E+04
400.00  -3.92294E+01  -9.61533E+04  -2.10482E+02  -1.19604E+04
500.00  -3.34122E+01  -9.97861E+04  -2.18613E+02  9.52022E+03
600.00  -2.77768E+01  -1.02842E+05  -2.24200E+02  3.16779E+04
700.00  -2.26324E+01  -1.05358E+05  -2.28088E+02  5.43040E+04
800.00  -1.81080E+01  -1.07390E+05  -2.30808E+02  7.72568E+04
900.00  -1.41889E+01  -1.09000E+05  -2.32710E+02  1.00438E+05
1000.00 -1.08095E+01  -1.10245E+05  -2.34025E+02  1.23779E+05
1100.00 -7.77802E+00  -1.11169E+05  -2.34908E+02  1.47229E+05
1200.00 -5.07556E+00  -1.11807E+05  -2.35464E+02  1.70750E+05
1300.00 -2.93467E+00  -1.12203E+05  -2.35782E+02  1.94314E+05
1400.00 -1.19414E+00  -1.12407E+05  -2.35934E+02  2.17901E+05
1500.00 2.55400E-01  -1.12452E+05  -2.35966E+02  2.41497E+05
1600.00 1.49022E+00  -1.12363E+05  -2.35909E+02  2.65091E+05
1700.00 2.56484E+00  -1.12159E+05  -2.35785E+02  2.88676E+05
1800.00 3.51909E+00  -1.11854E+05  -2.35611E+02  3.12246E+05
1900.00 4.38259E+00  -1.11458E+05  -2.35397E+02  3.35797E+05
2000.00 5.17775E+00  -1.10980E+05  -2.35152E+02  3.59325E+05

```

TAB:Hit RETURN to continue

TAB: @@ Add a final column with a function. In this function

TAB: @@ you may use G, S, H, V, CP, T and R with their obvious

TAB: @@ meaning. You may also use H298 and ALPHA (thermal expansivity)

TAB: @@ and KAPPA (isothermal compressibility). In most databases

TAB: @@ there are no pressure dependence and thus V, ALPHA and KAPPA

TAB: @@ will not be correct.

TAB: e-fun

... the command in full is ENTER\_FUNCTION

Name: fef

Function: (g-h298)/t

&

TAB: t-r

... the command in full is TABULATE\_REACTION

Same reaction? /Y/: y  
Pressure /100000/: 100000  
Low temperature limit /298.15/: 298.15  
High temperature limit /2000/: 2000  
Step in temperature /100/: 100

Output file /SCREEN/:

O U T P U T F R O M T H E R M O - C A L C  
2016. 5.16 13.24.37

Column 6: fef (G-H298 )/T  
Reaction: 3H2<G>+N2<G>=2H3N1<G>  
H2<GAS>  
N2<GAS>  
H3N1<GAS>

T (K)	Delta-Cp (Joule/K)	Delta-H (Joule)	Delta-S (Joule/K)	Delta-G (Joule)	fef
298.15	-4.44006E+01	-9.18800E+04	-1.98115E+02	-3.28120E+04	1.98115E+02
300.00	-4.43267E+01	-9.19621E+04	-1.98389E+02	-3.24452E+04	1.98116E+02
400.00	-3.92294E+01	-9.61533E+04	-2.10482E+02	-1.19604E+04	1.99799E+02
500.00	-3.34122E+01	-9.97861E+04	-2.18613E+02	9.52022E+03	2.02800E+02
600.00	-2.77768E+01	-1.02842E+05	-2.24200E+02	3.16779E+04	2.05930E+02
700.00	-2.26324E+01	-1.05358E+05	-2.28088E+02	5.43040E+04	2.08834E+02
800.00	-1.81080E+01	-1.07390E+05	-2.30808E+02	7.72568E+04	2.11421E+02
900.00	-1.41889E+01	-1.09000E+05	-2.32710E+02	1.00438E+05	2.13687E+02
1000.00	-1.08095E+01	-1.10245E+05	-2.34025E+02	1.23779E+05	2.15659E+02
1100.00	-7.77802E+00	-1.11169E+05	-2.34908E+02	1.47229E+05	2.17372E+02
1200.00	-5.07556E+00	-1.11807E+05	-2.35464E+02	1.70750E+05	2.18858E+02
1300.00	-2.93467E+00	-1.12203E+05	-2.35782E+02	1.94314E+05	2.20149E+02
1400.00	-1.19414E+00	-1.12407E+05	-2.35934E+02	2.17901E+05	2.21272E+02
1500.00	2.55400E-01	-1.12452E+05	-2.35966E+02	2.41497E+05	2.22251E+02
1600.00	1.49022E+00	-1.12363E+05	-2.35909E+02	2.65091E+05	2.23107E+02
1700.00	2.56484E+00	-1.12159E+05	-2.35785E+02	2.88676E+05	2.23857E+02
1800.00	3.51909E+00	-1.11854E+05	-2.35611E+02	3.12246E+05	2.24515E+02
1900.00	4.38259E+00	-1.11458E+05	-2.35397E+02	3.35797E+05	2.25093E+02
2000.00	5.17775E+00	-1.10980E+05	-2.35152E+02	3.59325E+05	2.25602E+02

TAB:Hit RETURN to continue  
TAB: t-r  
... the command in full is TABULATE\_REACTION  
Same reaction? /Y/: y  
Pressure /100000/: 100000  
Low temperature limit /298.15/: 298.15  
High temperature limit /2000/: 2000  
Step in temperature /100/: 100

Output file /SCREEN/: tcex12a  
Grapical output? /Y/: y  
Plot column? /2/: 6

O U T P U T F R O M T H E R M O - C A L C  
2016. 5.16 13.24.37

Column 6: fef (G-H298 )/T  
Reaction: 3H2<G>+N2<G>=2H3N1<G>  
H2<GAS>  
N2<GAS>  
H3N1<GAS>

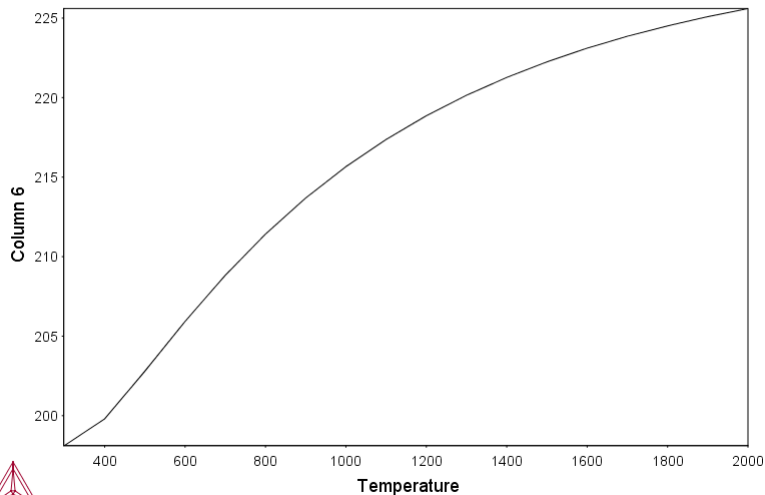
T (K)	Delta-Cp (Joule/K)	Delta-H (Joule)	Delta-S (Joule/K)	Delta-G (Joule)	fef
298.15	-4.44006E+01	-9.18800E+04	-1.98115E+02	-3.28120E+04	1.98115E+02
300.00	-4.43267E+01	-9.19621E+04	-1.98389E+02	-3.24452E+04	1.98116E+02
400.00	-3.92294E+01	-9.61533E+04	-2.10482E+02	-1.19604E+04	1.99799E+02
500.00	-3.34122E+01	-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



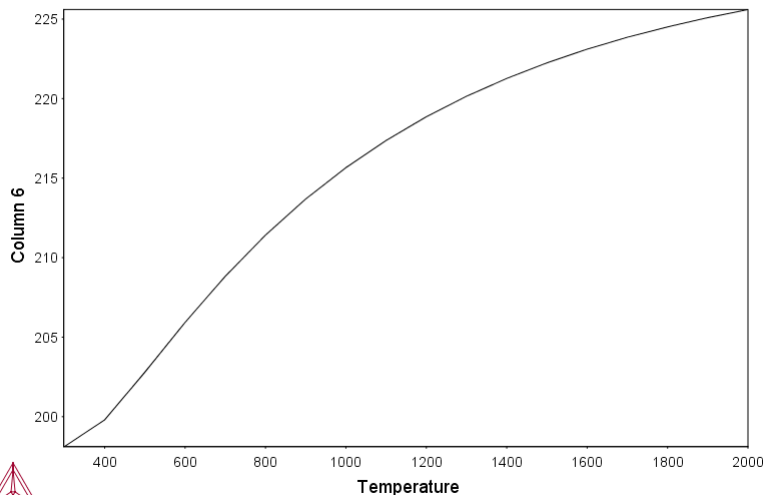
# REACTION TABULATION

2016.05.16.13.24.40  
SSUB5: H,N



POST:  
POST: set-title example 12a  
POST: plot  
... the command in full is PLOT DIAGRAM  
**example 12a**

2016.05.16.13.24.41  
SSUB5: H,N



POST:  
POST: Hit RETURN to continue  
POST: back  
TAB:  
TAB:  
TAB: @@ In the Gibbs-Energy-System we can list the data we use  
TAB: go g  
... the command in full is GOTO\_MODULE  
GIBBS ENERGY SYSTEM version 5.2  
GES: l-d  
... the command in full is LIST\_DATA  
OUTPUT TO SCREEN OR FILE /SCREEN/:  
OPTIONS?: ?

OPTIONS?

Choose one or several of the following options for output:  
\* N the output is written as a "user" database format.  
\* P the output is written as a MACRO file for future input.  
This is useful for creating setup files for assessments.  
\* S the symbols are suppressed.  
\* R the references for the parameters are listed  
(only for some databases in which references are available)  
\* L the output is written suitable for a LaTeX preprocessor.

OPTIONS?: rs

1 OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT DATE 2016- 5-16  
FROM DATABASE: SSUB5

ALL DATA IN SI UNITS  
FUNCTIONS VALID FOR 298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

ELEMENT	TABLE	ELEMENT	REFERENCE	MASS	H298-H0	S298
0	VA	VACUUM		0.0000E+00	0.0000E+00	0.0000E+00
1	H	1/2_MOLE_H2 (GAS)		1.0079E+00	4.2340E+03	6.5285E+01
2	N	1/2_MOLE_N2 (GAS)		1.4007E+01	4.3350E+03	9.5751E+01

SPECIES	STOICHIOMETRY
1 H	H
2 H2	H2

```
3 H3N1          H3N1
4 N             N
5 N2            N2
6 VA            VA
```

GAS

CONSTITUENTS: H2,H3N1,N2

```
G(GAS,H2;0)- 2 H298 (1/2_MOLE_H2(GAS),H;0) = +F11227T+R*T*LN(1E-05*P)
REFERENCE: 9480
G(GAS,H3N1;0)- 3 H298 (1/2_MOLE_H2(GAS),H;0)-H298 (1/2_MOLE_N2(GAS),N;0)
= +F11369T+R*T*LN(1E-05*P)
REFERENCE: 9537
G(GAS,N2;0)- 2 H298 (1/2_MOLE_N2(GAS),N;0) = +F13668T+R*T*LN(1E-05*P)
REFERENCE:11534
```

LIST OF REFERENCES

NUMBER SOURCE

```
REF9480 H2<G> JANAF THERMOCHEMICAL TABLES SGTE **
H2<G> H2<G>
HYDROGEN<G>
STANDARD STATE FROM CODATA KEY VALUES. CP FROM JANAF PUB. 3/61
REF9537 H3N1<G> T.C.R.A.S. Class: 2
H3N1<G> NH3<G>
AMMONIA <GAS>
REF11534 N2<G> JANAF THERMOCHEMICAL TABLES SGTE **
N2<G> N2<G>
NITROGEN <DIATOMIC GAS>
PUBLISHED BY JANAF AT 09/65
```

GES:Hit RETURN to continue

GES: back

TAB:

TAB: @@ Tabulate another reaction =====

TAB: t-r

... the command in full is TABULATE\_REACTION

Same reaction? /Y/: n

Reaction: INP+GA=GAP+IN;

... the command in full is REJECT

VA DEFINED

REINITIATING GES5 .....

... the command in full is DEFINE\_SPECIES

GA IN1P1 IN

GA1P1 DEFINED

... the command in full is GET\_DATA

ELEMENTS .....

SPECIES .....

PHASES .....

PARAMETERS ...

FUNCTIONS ....

List of references for assessed data

```
GA1<G> T.C.R.A.S. Class: 1
GA1<G> Ga<G>
GALLIUM <GAS>
GA1P1<G> S.G.T.E.
GA1P1<G> GaP<G>
GALLIUM PHOSPHIDE <GAS>
ASSESSED DATA BY C. CHATILLON MARCH 1994. Ga(g) and P2(g)
from T.C.R.A.S.
IN1<G> THERMODATA
IN1<G> In<G>
New Assessment (H form and S only)
IN1P1<G> CHATILLON(1994 March)
IN1P1<G> InP<G>
ASSESSED DATA BY C. CHATILLON MARCH 1994. In(g) and P2(g)
from T.C.R.A.S.
GA1P1 S.G.T.E.
GA1P1 GaP
GALLIUM PHOSPHIDE. Calphad, 18, 2, 177-222 (1994).
GA1 S.G.T.E. **
GA1 Ga
GALLIUM
Data from SGTE Unary DB , based on 81GLU/GUR (Ivtan Vol. 3)
20080211 BC Tref 200 -> 298.15
IN1P1 I. BARIN 3rd. Edition
IN1P1 InP
INDIUM MONOPHOSPHIDE. Data taken from Calphad, 18, 2, 177-222
(1994)
IN1 S.G.T.E. **
IN1 In
INDIUM
Data from SGTE Unary DB
```

-OK-

Pressure /100000/: 100000

Low temperature limit /298.15/: 298.15

High temperature limit /2000/: 2000

Step in temperature /100/: 100

Output file /tcex12a/: tcex12b

Graphical output? /Y/: Y

Plot column? /2/: 2

```
O U T P U T   F R O M   T H E R M O - C A L C
2016. 5.16                                13.24.41
```

Column 6: fef (G-H298 )/T

Reaction: GA+IN1P1=IN+GA1P1

GA stable as GA\_S

IN1P1 stable as IN1P1\_S

IN stable as IN\_S

GA1P1 stable as GA1P1\_S

```
*****
T      Delta-Cp      Delta-H      Delta-S      Delta-G      fef
(K)    (Joule/K)     (Joule)    (Joule/K)    (Joule)
*****
298.15 -1.56785E+00 -4.01610E+04  4.46600E+00 -4.14925E+04 -4.46600E+00
300.00 -1.60915E+00 -4.01639E+04  4.45617E+00 -4.15008E+04 -4.46597E+00
302.    ---- GA becomes GA_L,delta-H = 5589.80
400.00 -6.09329E-01 -4.59820E+04 -1.46756E+01 -4.01118E+04  1.23002E-01
*****
```

```

430.  ---- IN becomes IN_L ,delta-H = 3283.00
500.00  7.26020E-01  -4.26605E+04  -6.95385E+00  -3.91835E+04  1.95492E+00
600.00  1.12393E+00  -4.25671E+04  -6.78469E+00  -3.84963E+04  2.77457E+00
700.00  1.32655E+00  -4.24423E+04  -6.59282E+00  -3.78274E+04  3.33376E+00
800.00  1.22407E+00  -4.23120E+04  -6.41862E+00  -3.71771E+04  3.72988E+00
900.00  7.64029E-01  -4.22095E+04  -6.29733E+00  -3.65419E+04  4.02125E+00
1000.00 -8.12013E-02  -4.21720E+04  -6.25712E+00  -3.59149E+04  4.24608E+00
1100.00 -1.32730E+00  -4.22391E+04  -6.32007E+00  -3.52870E+04  4.43091E+00
1200.00 -2.98369E+00  -4.24512E+04  -6.50358E+00  -3.46469E+04  4.59509E+00
Temperature range exceeded for IN1P1

```

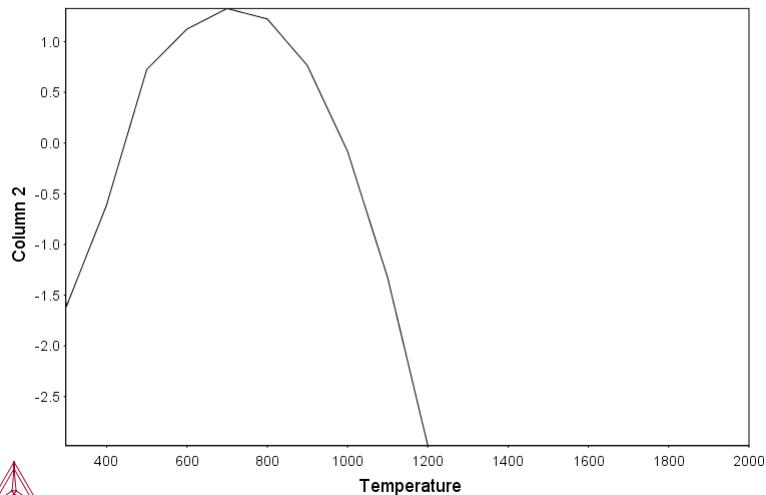
```

... the command in full is QUICK_EXPERIMENTAL_PLOT
... the command in full is SET_SCALING_STATUS
... the command in full is PLOT DIAGRAM

```

## REACTION TABULATION

2016.05.16.13.24.41  
SSUB5: GA, IN, P



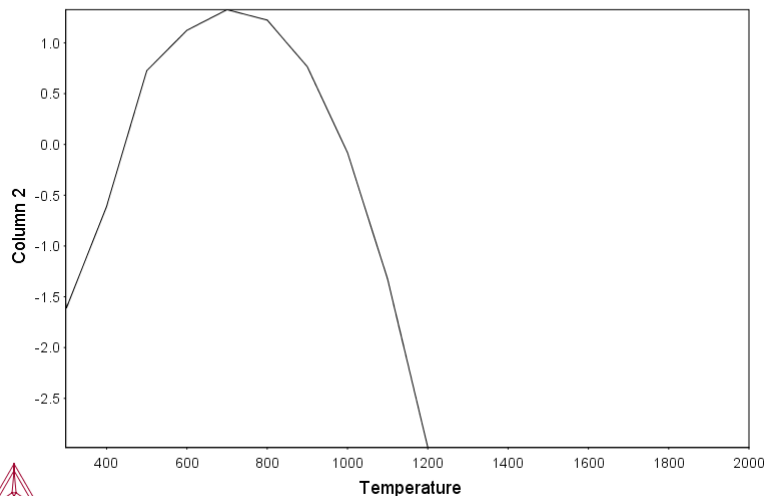
```

POST:
POST: set-title example 12b
POST:
POST: plot
... the command in full is PLOT DIAGRAM

```

## example 12b

2016.05.16.13.24.41  
SSUB5: GA, IN, P



```

POST:
POST:Hit RETURN to continue
POST: back
TAB:
TAB:
TAB: @@ By default a species in a gas is not included in
TAB: @@ a tabulation, you must specify <GAS> if you want that
TAB: t-r n
... the command in full is TABULATE_REACTION
Reaction: INP<gas>+GA=GAP+IN;
... the command in full is REJECT
VA DEFINED
REINITIATING GES5 .....
... the command in full is DEFINE_SPECIES
GA IN1P1 IN
GA1P1 DEFINED
... the command in full is GET_DATA
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

```

List of references for assessed data

```

GA1<G> T.C.R.A.S. Class: 1
GA1<G> Ga<G>
GALLIUM <GAS>
GA1P1<G> S.G.T.E.
GA1P1<G> GaP<G>

```

```
GALLIUM PHOSPHIDE <GAS>
ASSESSED DATA BY C. CHATILLON MARCH 1994. Ga(g) and P2(g)
from T.C.R.A.S.
IN1<G> THERMODATA
IN1<G> In<G>
New Assessment (H form and S only)
IN1P1<G> CHATILLON(1994 March)
IN1P1<G> InP<G>
ASSESSED DATA BY C. CHATILLON MARCH 1994. In(g) and P2(g)
from T.C.R.A.S.
GA1P1 S.G.T.E.
GA1P1 GaP
GALLIUM PHOSPHIDE. Calphad, 18, 2, 177-222 (1994).
GA1 S.G.T.E. **
GA1 Ga
GALLIUM
Data from SGTE Unary DB , based on 81GLU/GUR (Ivtan Vol. 3)
20080211 BC Tref 200 -> 298.15
IN1P1 I. BARIN 3rd. Edition
IN1P1 InP
INDIUM MONOPHOSPHIDE. Data taken from Calphad, 18, 2, 177-222
(1994)
IN1 S.G.T.E. **
IN1 In
INDIUM
Data from SGTE Unary DB
```

-OK-

Pressure /100000/: 100000

Low temperature limit /298.15/: 1000

High temperature limit /2000/: 2000

Step in temperature /100/: 100

Output file /tcex12b/:

Grapical output? /Y/: N

O U T P U T F R O M T H E R M O - C A L C  
2016. 5.16 13.24.42

Column 6: fef (G-H298 )/T

Reaction: GA+IN1P1<G>=IN+GA1P1

GA stable as GA\_L

IN1P1<GAS>

IN1P1<GAS>

IN stable as IN\_L

GA1P1 stable as GA1P1\_S

```
*****
T      Delta-Cp      Delta-H      Delta-S      Delta-G      fef
(K)    (Joule/K)      (Joule)    (Joule/K)    (Joule)
*****
1000.00 1.57503E+01 -4.65760E+05 -1.78780E+02 -2.86980E+05 1.86368E+02
1100.00 1.60263E+01 -4.64172E+05 -1.77266E+02 -2.69179E+05 1.85608E+02
1200.00 1.63030E+01 -4.62555E+05 -1.75860E+02 -2.51523E+05 1.84854E+02
1300.00 1.65828E+01 -4.60911E+05 -1.74544E+02 -2.34004E+05 1.84111E+02
1400.00 1.68674E+01 -4.59238E+05 -1.73305E+02 -2.16612E+05 1.83383E+02
1500.00 1.71578E+01 -4.57537E+05 -1.72131E+02 -1.99341E+05 1.82672E+02
1600.00 1.74548E+01 -4.55807E+05 -1.71014E+02 -1.82184E+05 1.81978E+02
1700.00 1.77582E+01 -4.54046E+05 -1.69947E+02 -1.65136E+05 1.81301E+02
Temperature range exceeded for GA1P1
```

TAB:Hit RETURN to continue

TAB: @@ =====

TAB: @@ You can list substances in the database

TAB: li-sub

... the command in full is LIST\_SUBSTANCES

... the command in full is REJECT

VA DEFINED

REINITIATING GES5 .....

... the command in full is DEFINE\_SPECIES

AG DEFINED

... the command in full is GET\_DATA

ELEMENTS .....

SPECIES .....

PHASES .....

PARAMETERS ...

FUNCTIONS ....

List of references for assessed data

AG1<G> THERMODATA

AG1<G> Ag<G>

SILVER <GAS>

Modified Thermodata new assessment

AG1 HULTGREN SELECTED VAL. SGTE \*\*

AG1 Ag

SILVER

CODATA KEY VALUE.MPT=1234.93K.

--U.D. 30/10/85 .

-OK-

With elements /\*/: IN P

Exclusivly with those elements? /Y/:

IN P IN2

IN1P1 P2 P3

P4

TAB: @@ or all substances with Fe

TAB: li-sub

... the command in full is LIST\_SUBSTANCES

With elements /\*/: FE

Exclusivly with those elements? /Y/: N

```
FE AL2FE1O4 AS1FE1O4
AS2FE3O8 B1FE1 B1FE2
BA1FE1ND1O4 BA1FE2ND2O7 BR1FE1
BR2FE1 BR3FE1 BR4FE2
BR6FE2 C1FE1O3 C1FE3
C5FE1O5 CA1FE2O4 CA2FE2O5
CD1FE2O4 CL1FE1 CL1FE1O1
CL2FE1 CL3FE1 CL4FE2
CL6FE2 CO1FE2O4 CR2FE1O4
CU1FE1O2 CU1FE1S2 CU1FE2O4
CU2FE2O4 CU5FE1S4 F1FE1
F2FE1 F3FE1 F4FE2
F6FE2 FE1/+1 FE1/-1
FE2 FE1H1 FE1H1O1
FE1H1O2 FE2H2O4 FE1H2O2
FE1H3O3 FE0.947O1 FE1O1
```

FE1O2	FE2O3	FE3O4
FE0.875S1	FE1S1	FE1S2
FE1O4S1	FE2O12S3	FE1SE0.96
FE1.04SE1	FE1SE1	FE1SE2
FE2N1	FE4N1	FE1P1
FE1P2	FE2P1	FE3P1
FE1H4O6P1	FE1I1	FE1I2
FE1I3	FE2I4	FE2I6
FE1K1O2	FE1K2O2	FE1K4O3
FE1LI1O2	FE1LI5O4	FE1MO1O4
FE1NA1O2	FE1O3S11	FE1O3TI1
FE1O4V2	FE1O4W1	FE1O6V2
FE1S11	FE1SI2.33	FE1SI2
FE1TE0.9	FE1TE1	FE1TE2
FE1TI1	FE2LI2O4	FE2MG1O4
FE2MN1O4	FE2NB1	FE2NI1O4
FE2O4S11	FE2O4TI1	FE2O4ZN1
FE2TA1	FE2TI1	FE2U1
FE3LI2O5	FE3MO2	FE3W2
FE5LI1O8		

TAB:

TAB:Hit RETURN to continue

TAB: @@ =====

TAB: @@ You can tabulate data for a substance or phase also, this is equivalent

TAB: @@ with tabels you may find in JANAF for example

TAB: t-sub IN1P1

... the command in full is TABULATE\_SUBSTANCE

... the command in full is REJECT

VA DEFINED

REINITIATING GES5 .....

... the command in full is DEFINE\_SPECIES

IN1P1 DEFINED

... the command in full is GET\_DATA

ELEMENTS .....

SPECIES .....

PHASES .....

PARAMETERS ...

FUNCTIONS ....

List of references for assessed data

IN1P1<G> CHATILLON(1994 March)

IN1P1<G> InP<G>

ASSESSED DATA BY C. CHATILLON MARCH 1994. In(g) and P2(g)

from T.C.R.A.S.

IN1P1 I. BARIN 3rd. Edition

IN1P1 InP

INDIUM MONOPHOSPHIDE. Data taken from Calphad, 18, 2, 177-222

(1994)

-OK-

Pressure /100000/: 100000

Low temperature limit /1000/: 300

High temperature limit /2000/: 1300

Step in temperature /100/: 100

Output file /tcex12b/: tcex12c

Grapical output? /Y/: Y

Plot column? /2/: 2

O U T P U T F R O M T H E R M O - C A L C  
2016. 5.16 13.24.42

Column 6: fef (G-H298 )/T

Phase : IN1P1\_S Pressure : 100000.00  
Specie: IN1P1

\*\*\*\*\*

T (K)	Cp (Joule/K)	H (Joule)	S (Joule/K)	G (Joule)	fef
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

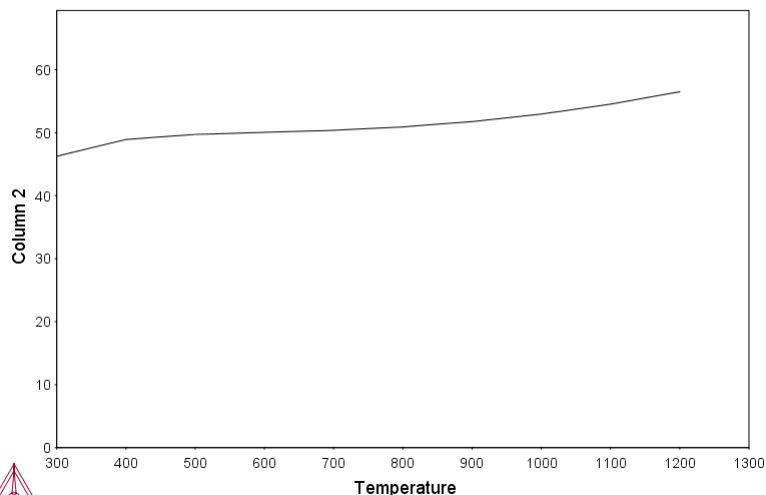
Temperature range exceeded

... the command in full is QUICK\_EXPERIMENTAL\_PLOT

... the command in full is PLOT\_DIAGRAM

# TABULATION FOR IN1P1\_S

2016.05.16.13.24.42  
SSUB5: IN, P



POST:Hit RETURN to continue

POST:

POST: set-title example 12c

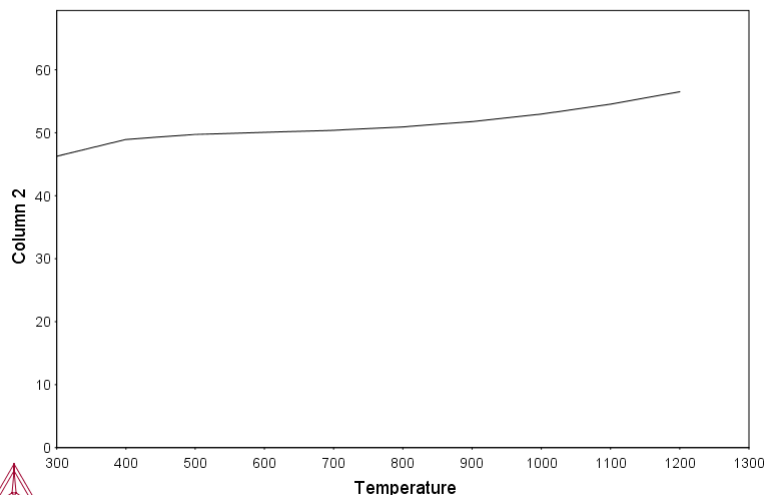
POST:

POST: plot

... the command in full is PLOT DIAGRAM

example 12c

2016.05.16.13.24.42  
SSUB5: IN, P



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 GES5 .....

... the command in full is DEFINE\_SPECIES

H1K1O1 DEFINED

... the command in full is GET\_DATA

ELEMENTS .....

SPECIES .....

PHASES .....

PARAMETERS ...

FUNCTIONS ....

List of references for assessed data

H1K1O1<G> J. Phys. Chem. Ref. Data

H1K1O1<G> KOH<G>

Data taken from JPCRD, 26, 4 1031-1110 (1997)

H1K1O1 J. Phys. Chem. Ref. Data

H1K1O1 KOH

Data taken from JPCRD, 26, 4 1031-1110 (1997)

-OK-

Pressure /100000/: 100000

Low temperature limit /300/: 300

High temperature limit /1300/: 2000

Step in temperature /100/: 100

Output file /tcex12c/: tcex12d  
Graphical output? /Y/: Y  
Plot column? /2/: 6

OUTPUT FROM THERMO - CALC  
2016. 5.16 13.24.42

Column 6: pp EXP(-G/R/T )  
Reaction: H1K1O1=H1K1O1<G>  
H1K1O1 stable as H1K1O1\_S  
H1K1O1<GAS>

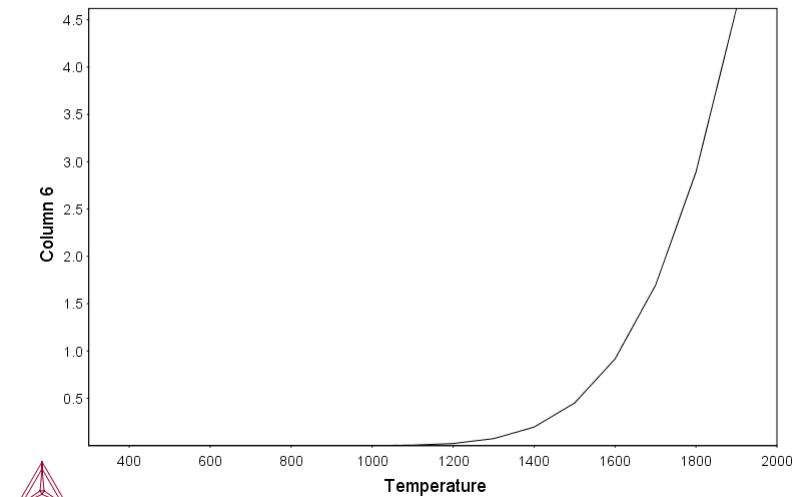
T (K)	Delta-Cp (Joule/K)	Delta-H (Joule)	Delta-S (Joule/K)	Delta-G (Joule)	pp
300.00	-1.97899E+01	1.92543E+05	1.56915E+02	1.45469E+05	4.70147E-26
400.00	-2.31294E+01	1.90409E+05	1.50797E+02	1.30090E+05	1.02900E-17
500.00	-2.73216E+01	1.87890E+05	1.45195E+02	1.15293E+05	9.03075E-13
517.	---- H1K1O1 becomes 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

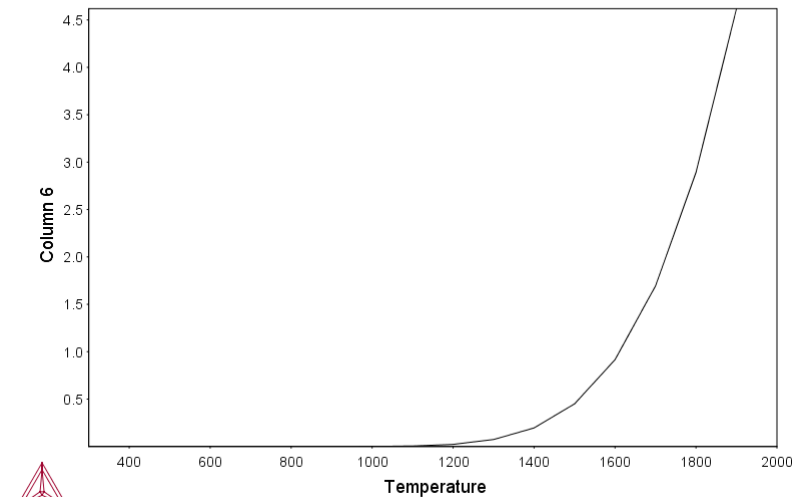
REACTION TABULATION

2016.05.16.13.24.43  
SSUBS: H,K,O



POST:  
POST: set-title example 12d  
POST:  
POST: plot  
... the command in full is PLOT DIAGRAM  
example 12d

2016.05.16.13.24.43  
SSUBS: H,K,O

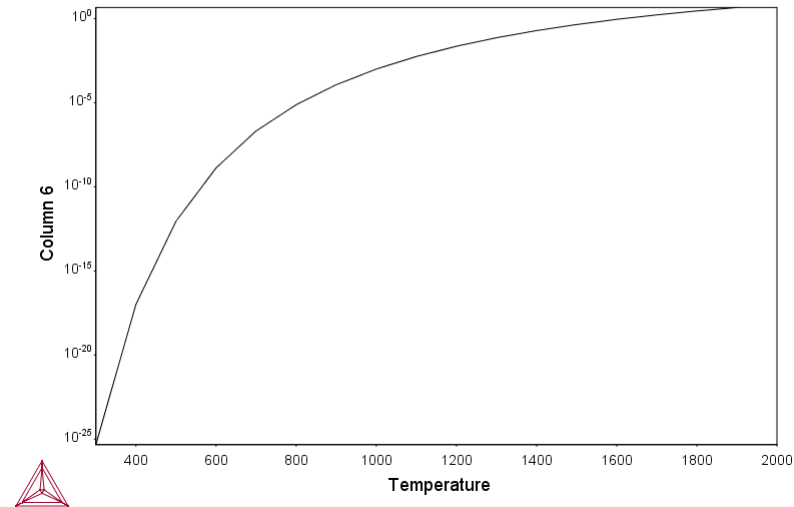


POST:  
POST:Hit RETURN to continue

```
POST: s-a-ty y
... the command in full is SET_AXIS_TYPE
AXIS TYPE /LINEAR/: log
POST: set-title example 12e
POST:
POST: plot
... the command in full is PLOT DIAGRAM
```

example 12e

2016.05.16.13.24.43  
SSUB5: H,K,O



```
POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:
```



## tcex13

### About

```
SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex13\tcex13.TCM"SYS: set-echo
SYS: @@
SYS: @@
SYS: @@ Calculation
SYS: @@ of phase diagram and G curve
SYS: @@ using the BINARY module
SYS: @@
SYS: @@ Binary Al-Ti phase diagram and G curve
SYS: @@
SYS: set-log ex13,,,
SYS: GO BIN
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v8.0
```

```
VA DEFINED
L12_FCC B2_BCC B2_VACANCY
HIGH_SIGMA DICTRA_FCC_A1 REJECTED
```

Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN

Current database: TC Binary Solutions v1.1

```
VA /- DEFINED
BCC_B2 FCC_L12 FCC_L102
D021_HCP REJECTED
```

First element: ?

The following assessed systems

```
AG-AL AG-AU AG-BI AG-CU AG-GE AG-IN AG-IR AG-MG AG-OS AG-PB AG-PD AG-PT
AG-RH AG-RU AG-SB AG-SI AG-SN AG-TI AG-TL AG-ZN AG-ZR AL-AS AL-AU AL-B
AL-BI AL-C AL-CA AL-CE AL-CO AL-CR AL-CU AL-FE AL-GA AL-GE AL-IN AL-LI
AL-MG AL-MN AL-MO AL-N AL-NB AL-ND AL-NI AL-O AL-P AL-PB AL-SB AL-SI
AL-SN AL-TA AL-TI AL-V AL-W AL-Y AL-ZN AL-ZR AS-AU AS-CU AS-FE AS-GA
AS-GE AS-IN AS-P AS-SB AU-BI AU-C AU-CR AU-CU AU-GE AU-IN AU-PB AU-PD
AU-RH AU-RU AU-SB AU-SI AU-TE AU-TL B-C B-CO B-CR B-FE B-HF B-MG
B-MO B-N B-ND B-NI B-SC B-SI B-TI B-V B-W BA-CU BA-EU BA-SR
BA-Y BI-CU BI-GA BI-GE BI-HG BI-IN BI-K BI-MG BI-O BI-PB BI-SB BI-SI
BI-SN BI-TL BI-ZN C-CO C-CR C-CU C-FE C-HF C-MN C-MO C-NB C-NI
C-PB C-SI C-TA C-TI C-V C-W C-Y C-ZR CA-CU CA-MG CA-PB CA-SI
CA-ZN CD-GA CD-GE CD-HG CD-IN CD-PB CD-SB CD-SN CD-TE CD-ZN CE-MG CO-CR
CO-CU CO-DY CO-FE CO-IN CO-MN CO-MO CO-N CO-NB CO-NI CO-PD CO-PT CO-SI
CO-TA CO-TI CO-V CO-W CR-CU CR-FE CR-MG CR-MN CR-MO CR-N CR-NB CR-NI
CR-P CR-PD CR-PT CR-SI CR-SN CR-TA CR-TI CR-V CR-W CR-ZN CR-ZR CS-K
CS-NA CS-RB CU-FE CU-GE CU-IN CU-LI CU-MG CU-MN CU-N CU-NB CU-NI CU-O
CU-P CU-PB CU-S CU-SB CU-SI CU-SN CU-SR CU-TI CU-TL CU-V CU-Y CU-ZN
CU-ZR DY-ER DY-HO ER-HO ER-TB FE-MG FE-MN FE-MO FE-N FE-NB FE-ND FE-NI
FE-O FE-P FE-PB FE-PD FE-PR FE-PT FE-S FE-SI FE-SN FE-TI FE-V FE-W
FE-ZN FE-ZR GA-GE GA-HG GA-IN GA-P GA-PB GA-SB GA-SN GA-TE GA-ZN GE-IN
GE-PB GE-SB GE-SI GE-SN GE-TE GE-TL GE-ZN H-NB H-ZR HF-TA HF-SI HF-TI
HG-PB HO-TB IN-P IN-PB IN-SB IN-SI IN-SN IN-ZN IR-PD K-RB LA-NI LI-MG
LI-ZR MG-MN MG-NI MG-O MG-SC MG-SI MG-Y MG-ZN MG-ZR MN-MO MN-N MN-O
MN-PB MN-SI MN-TI MN-V MN-Y MN-ZR MO-N MO-NB MO-NI MO-SI MO-TA MO-TI
MO-W N-NB N-NI N-TA N-TI N-V N-W NA-RB NB-NI NB-O NB-TI NB-V
NB-W NB-ZR ND-PR ND-SB NI-P NI-PD NI-SI NI-TA NI-TI NI-V NI-W NI-Y
NI-ZR O-PB O-SN O-SR O-TI O-Y O-ZR P-SB P-SI PB-PD PB-SB PB-SI
PB-SN PB-TL PB-ZN PD-RU PD-SN PR-SB PT-RH PT-RU RE-TA RE-W SB-SI SB-SN
SB-ZN SE-SN SE-TE SE-TL SI-SN SI-TA SI-TE SI-TI SI-U SI-V SI-W SI-Y
SI-ZN SI-ZR SN-TI SN-ZN SN-ZR TA-TI TA-V TA-W TA-ZR TE-ZN TI-V TI-W
TI-ZR U-ZR V-ZR Y-ZR
```

First element: AL TI

Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase\_Diagram/:

```
... the command in full is REJECT
VA /- DEFINED
BCC_B2 FCC_L12 FCC_L102
D021_HCP REJECTED
REINITIATING GES5 .....
... the command in full is DEFINE_ELEMENTS
AL TI DEFINED
GAS:G LIQUID:L IONIC_LIQUID:Y
FCC_A1 BCC_A2 A2_BCC
HCP_A3 HCP_ZN DIAMOND_A4
BCT_A5 CBCC_A12 CUB_A13
B11_CUT1 B32_ALL1 C14_LAVES
C15_LAVES C16_AL2CU C36_LAVES
D019_AL1M3 D019_SNTI3 D022_AL3M1
D1A_CU4TI D513_AL3NI2 D88_S13TI5
L10_ALTI AL11TI5 AL2TI
AL5FE4 ALCE_AMORPHOUS MTI2
REJECTED
LIQUID:L RESTORED
AL11TI5 RESTORED
AL2TI RESTORED
D022_AL3M1 RESTORED
D019_AL1M3 RESTORED
L10_ALTI RESTORED
A2_BCC RESTORED
BCC_B2 RESTORED
FCC_A1 RESTORED
HCP_A3 RESTORED
... the command in full is GET_DATA
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....
```

List of references for assessed data

```
'A T Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4 p 317-425; '
'A T Dinsdale, SGTE Data for Pure Elements, update 2001'
'N Saunders, COST 507 (1998) ISBN 92-828-3902-8 p 89-94; Al-Ti'
'N. Dupin, 1999, lattice stability for G(BCC_A2,VA:VA)'
'N. Dupin, I. Ansara, Z. metallkd., Vol 90 (1999) p 76-85; Al-Ni'
'A V Davydov et al, Metall Mater Trans 32A (2001)9 p 2175-2186; Co-Ti'
```

```

'B Sundman, fix to avoid BCC with just Va (2001)'
'B Sundman, Set to zero due to the phase partitioning model '
-OK-
... the command in full is SET_AXIS_VARIABLE
The condition X(TI)=.1234 created
... the command in full is SET_AXIS_VARIABLE
The condition T=1319.08 created
... the command in full is SET_REFERENCE_STATE
... the command in full is SET_REFERENCE_STATE
... the command in full is SAVE_WORKSPACES
... the command in full is SET_CONDITION
... the command in full is SET_ALL_START_VALUES
Forcing automatic start values
Automatic start values will be set
... the command in full is COMPUTE_EQUILIBRIUM
... the command in full is COMPUTE_EQUILIBRIUM
Start points provided by database
... the command in full is SAVE_WORKSPACES
Version S mapping is selected

Organizing start points

Generating start point 1
Generating start point 2

Phase region boundary 1 at: 4.169E-01 1.704E+03
LIQUID
** L10_ALTI
Calculated. 7 equilibria

Phase region boundary 2 at: 3.454E-01 1.652E+03
LIQUID
** AL11TI5
** L10_ALTI

Phase region boundary 3 at: 3.153E-01 1.652E+03
LIQUID
** AL11TI5
Calculated. 3 equilibria

Phase region boundary 4 at: 3.016E-01 1.646E+03
LIQUID
** AL11TI5
** D022_AL3M1

Phase region boundary 5 at: 2.797E-01 1.646E+03
LIQUID
** D022_AL3M1
Calculated. 36 equilibria

Phase region boundary 6 at: 1.254E-01 9.380E+02
LIQUID
** D022_AL3M1
** FCC_A1

Phase region boundary 7 at: 4.025E-03 9.380E+02
LIQUID
** FCC_A1
Calculated 12 equilibria

Phase region boundary 8 at: 1.287E-01 9.380E+02
D022_AL3M1
** FCC_A1
Calculated.. 27 equilibria
Terminating at axis limit.

Phase region boundary 9 at: 2.981E-01 1.646E+03
AL11TI5
** D022_AL3M1
Calculated. 17 equilibria

Phase region boundary 10 at: 2.871E-01 1.269E+03
AL11TI5
** AL2TI
** D022_AL3M1

Phase region boundary 11 at: 3.267E-01 1.269E+03
AL11TI5
** AL2TI
Calculated. 9 equilibria

Phase region boundary 12 at: 3.267E-01 1.454E+03
AL11TI5
** AL2TI
** L10_ALTI

Phase region boundary 13 at: 3.539E-01 1.454E+03
AL11TI5
** L10_ALTI
Calculated. 9 equilibria
Terminating at known equilibrium

Phase region boundary 14 at: 3.605E-01 1.454E+03
AL2TI
** L10_ALTI
Calculated.. 48 equilibria
Terminating at axis limit.

Phase region boundary 15 at: 2.937E-01 1.269E+03
** AL2TI
D022_AL3M1
Calculated.. 40 equilibria
Terminating at axis limit.

Phase region boundary 16 at: 3.454E-01 1.652E+03
LIQUID
** L10_ALTI
Calculated. 9 equilibria

Phase region boundary 17 at: 4.476E-01 1.717E+03
LIQUID
** HCP_A3
** L10_ALTI

Phase region boundary 18 at: 4.672E-01 1.717E+03
LIQUID

```

```

** HCP_A3
Calculated.                4 equilibria

Phase region boundary 19 at: 5.157E-01 1.776E+03
LIQUID
** BCC_B2
** HCP_A3

Phase region boundary 20 at: 5.233E-01 1.776E+03
LIQUID
** BCC_B2
Calculated                43 equilibria

Phase region boundary 21 at: 5.477E-01 1.776E+03
** BCC_B2
HCP_A3
Calculated                41 equilibria

Phase region boundary 22 at: 4.784E-01 1.717E+03
** HCP_A3
L10_ALTI
Calculated.                14 equilibria

Phase region boundary 23 at: 5.545E-01 1.399E+03
** D019_AL1M3
** HCP_A3
L10_ALTI

Phase region boundary 24 at: 5.596E-01 1.399E+03
** D019_AL1M3
L10_ALTI
Calculated..              45 equilibria
Terminating at axis limit.

Phase region boundary 25 at: 5.977E-01 1.399E+03
** D019_AL1M3
HCP_A3
Calculated..              63 equilibria
Terminating at axis limit.

Phase region boundary 26 at: 4.169E-01 1.704E+03
LIQUID
** L10_ALTI
Calculated.                4 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex13\BINA
RY.POLY3
CPU time for mapping                2 seconds

```

POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

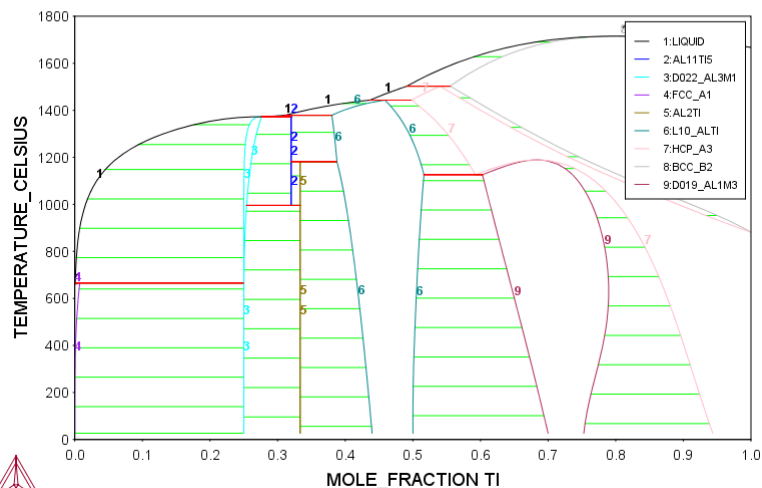
```

... the command in full is SET_TIELINE_STATUS
... the command in full is SET_LABEL_CURVE_OPTION
... the command in full is PLOT_DIAGRAM

```

AL TI

2016.05.16.13.26.57  
TCBIN:AL,TI  
P=1E5,N=1



POST: @@ Set some phase labels

POST: ADD

... the command in full is ADD\_LABEL\_TEXT

Give X coordinate in axis units: .7 1400

Automatic phase labels? /Y/:

Automatic labelling not always possible

Using global minimization procedure

Calculated 5763 grid points in 0 s

Found the set of lowest grid points in 0 s

Calculated POLY solution 1 s, total time 1 s

Stable phases are: BCC\_B2

Text size: /.36/: ADD

\*\*\* ERROR 1034 IN GETREL

\*\*\* NO DIGIT

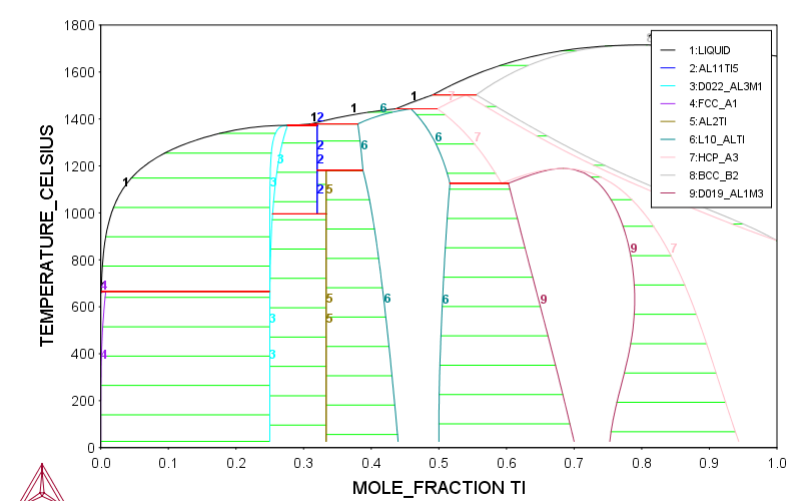
POST: .51 400

No such command, use HELP

POST:

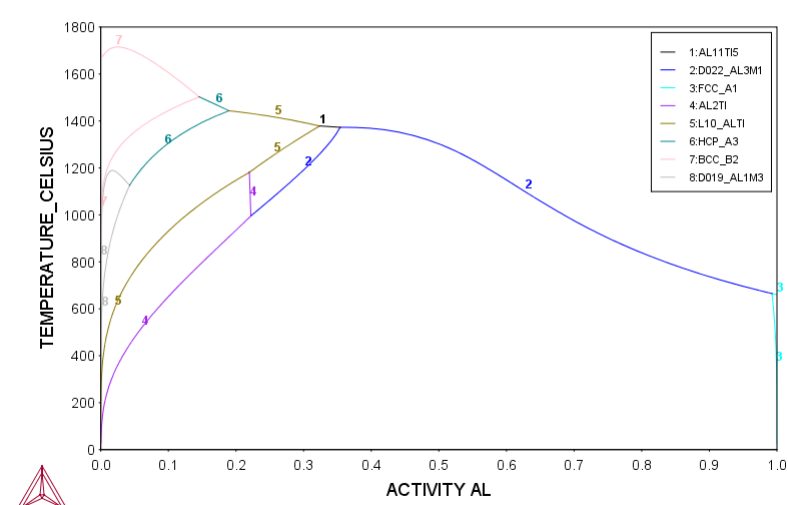
POST: set-title example 13a  
POST: plot  
... the command in full is PLOT DIAGRAM  
example 13a

2016.05.16.13.26.58  
TCBIN: AL, TI  
P=1E5, N=1



POST:  
POST:Hit RETURN to continue  
POST: @@ We may plot the activites as well  
POST: S-D-A  
... the command in full is SET\_DIAGRAM\_AXIS  
AXIS (X, Y OR Z) : X  
VARIABLE : AC  
FOR COMPONENT : AL  
POST: s-l e  
... the command in full is SET\_LABEL\_CURVE\_OPTION  
POST: set-title example 13b  
POST:  
POST: plot  
... the command in full is PLOT DIAGRAM  
example 13b

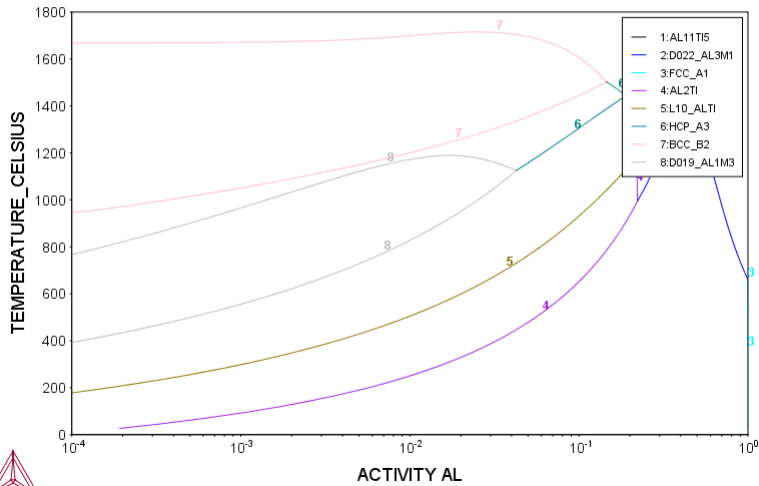
2016.05.16.13.26.59  
TCBIN: AL, TI  
P=1E5, N=1



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

### example 13c

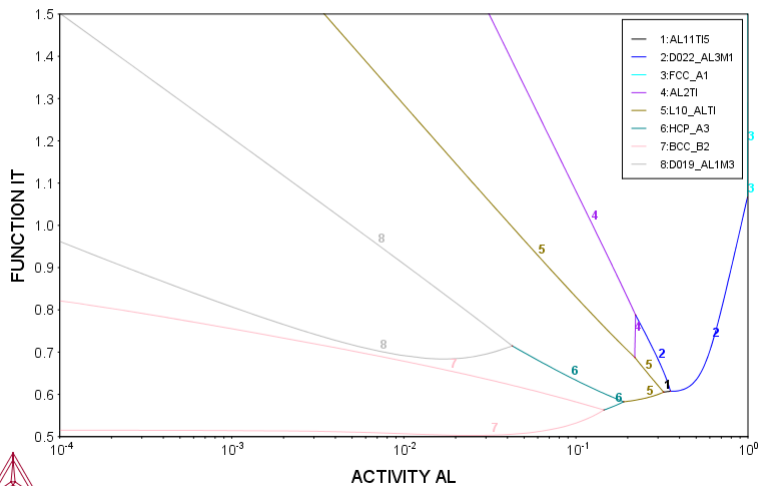
2016.05.16.13.26.59  
TCBIN: AL, TI  
P=1E5, N=1



```
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
```

### example 13d

2016.05.16.13.26.59  
TCBIN: AL, TI  
P=1E5, N=1



```
POST:
POST:Hit RETURN to continue
POST: @@ Now the G curves for the same system
POST: BA
... the command in full is BACK
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
L12_FCC          B2_BCC          B2_VACANCY
HIGH_SIGMA      DICTRA_FCC_A1   REJECTED
SYS: GO BIN
... the command in full is GOTO_MODULE
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
L12_FCC          B2_BCC          B2_VACANCY
HIGH_SIGMA      DICTRA_FCC_A1   REJECTED

Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN
Current database: TC Binary Solutions v1.1

VA          /- DEFINED
BCC_B2      FCC_L12          FCC_L102
D021_HCP    REJECTED
First element: AL TI
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/: G
Temperature (C): /1000/: 1000
... the command in full is REJECT
VA          /- DEFINED
BCC_B2      FCC_L12          FCC_L102
D021_HCP    REJECTED
REINITIATING GES5 .....
... the command in full is DEFINE_ELEMENTS
```

```

AL          TI   DEFINED
GAS:G       LIQUID:L          IONIC_LIQUID:Y
FCC_A1      BCC_A2           A2_BCC
HCP_A3      HCP_ZN           DIAMOND_A4
BCT_A5      CBCC_AL2        CUB_A13
B11_CUTI    B32_ALLI        C14_LAVES
C15_LAVES   C16_AL2CU        C36_LAVES
D019_AL1M3  D019_SNTI3       D022_AL3M1
D1A_CU4TI   D513_AL3NI2      D88_SI3TI5
L10_ALTI    AL11TI5          AL2TI
AL5FE4      ALCE_AMORPHOUS    MTI2

REJECTED
LIQUID:L    RESTORED
AL11TI5     RESTORED
AL2TI       RESTORED
D022_AL3M1  RESTORED
D019_AL1M3  RESTORED
L10_ALTI    RESTORED
A2_BCC      RESTORED
BCC_B2      RESTORED
FCC_A1      RESTORED
HCP_A3      RESTORED
... the command in full is GET_DATA
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

'A T Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4 p 317-425; '
'A T Dinsdale, SGTE Data for Pure Elements, update 2001'
'N Saunders, COST 507 (1998) ISBN 92-828-3902-8 p 89-94; Al-Ti'
'N. Dupin, 1999, lattice stability for G(BCC_A2,VA:VA)'
'N. Dupin, I. Ansara, Z. metallkd., Vol 90 (1999) p 76-85; Al-Ni'
'A V Davydov et al, Metall Mater Trans 32A (2001)9 p 2175-2186; Co-Ti'
'B Sundman, fix to avoid BCC with just Va (2001)'
'B Sundman, Set to zero due to the phase partitioning model '
-OK-
... the command in full is SET_AXIS_VARIABLE
The condition X(TI)=.1234 created
... the command in full is SET_CONDITION
... the command in full is COMPUTE_EQUILIBRIUM
... the command in full is SET_REFERENCE_STATE
... the command in full is SET_REFERENCE_STATE
... the command in full is SAVE_WORKSPACES
... the command in full is SET_ALL_START_VALUES
Forcing automatic start values
Automatic start values will be set
... the command in full is COMPUTE_EQUILIBRIUM
... the command in full is COMPUTE_EQUILIBRIUM
... the command in full is SAVE_WORKSPACES
... the command in full is STEP_WITH_OPTIONS

Phase Region from 0.502463 for:
LIQUID
BCC_B2
D019_AL1M3
FCC_A1
HCP_A3
L10_ALTI

Phase Region from 0.502463 for:
LIQUID
BCC_B2
D019_AL1M3
FCC_A1
HCP_A3
L10_ALTI

Phase Region from 0.320000 for:
AL11TI5

Phase Region from 0.333333 for:
AL2TI

Phase Region from 0.636878 for:
D022_AL3M1

Phase Region from 0.636878 for:
D022_AL3M1
*** Buffer saved on file ***
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex13\GCUR
VE.POLY3

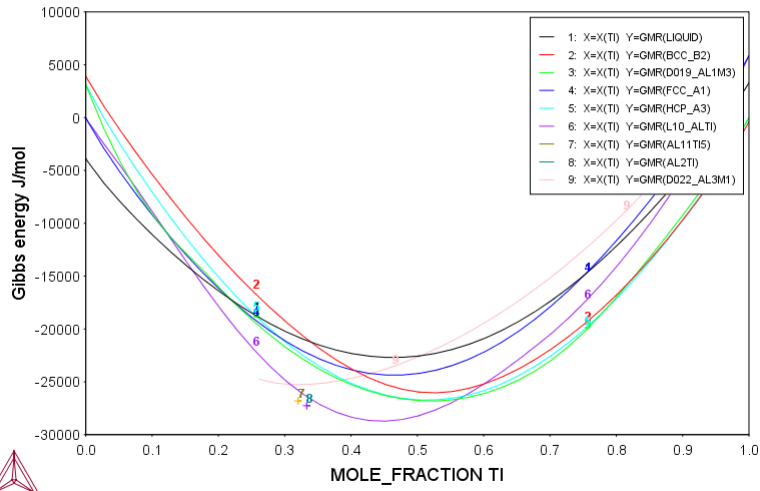
POSTPROCESSOR VERSION 3.2

... the command in full is SET_TIELINE_STATUS
... the command in full is SET_LABEL_CURVE_OPTION
... the command in full is PLOT_DIAGRAM

```

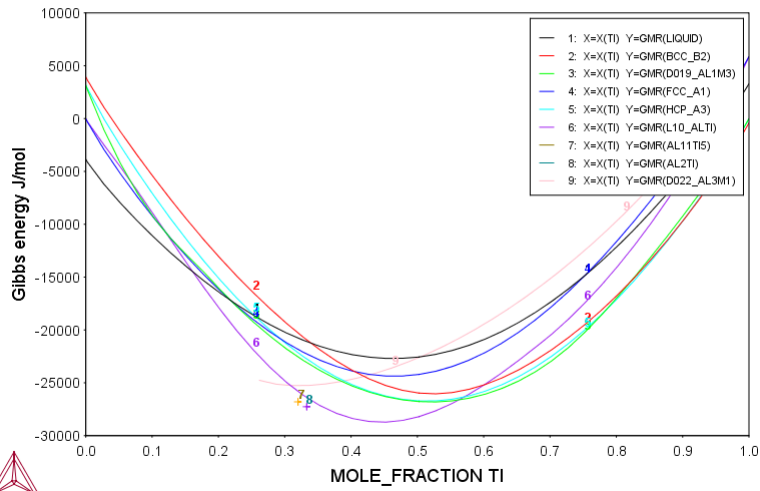
# AL TI

2016.05.16.13.27.06  
TCBIN: AL\_Ti  
P=1E5, N=1, T=1273.15



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  
example 13e

2016.05.16.13.27.06  
TCBIN: AL\_Ti  
P=1E5, N=1, T=1273.15



POST: set-inter  
... the command in full is SET\_INTERACTIVE\_MODE  
POST:

## tcex14

About License library version: 8.5.1.0017  
Linked: Mon May 16 09:31:44 2016

```
SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex14\tcex14.TCM" set-echo
SYS: @@
SYS: @@
SYS: @@ Calculation of the variation of the heat and the heat capacity
SYS: @@ during solidification of an Al-Cu-Si alloy
SYS: @@
SYS: set-log ex14,,,,,
SYS: go da
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
L12 FCC B2_BCC B2_VACANCY
HIGH_SIGMA DICTRA_FCC_A1 REJECTED
TDB_TCFE8: sw ALDEMO
... the command in full is SWITCH_DATABASE
Current database: Aluminum Demo Database

VA /- DEFINED
TDB_ALDEMO: d-sys al cu si
... the command in full is DEFINE_SYSTEM
AL CU SI
DEFINED
TDB_ALDEMO: l-s c
... the command in full is LIST_SYSTEM
LIQUID :AL CU SI:
HCP_A3 :AL CU SI:VA:
BCC_A2 :AL CU SI:VA:
BCC_B2 :AL CU SI:AL CU SI:VA:
FCC_A1 :AL CU SI:VA:
FCC_L12 :AL CU SI:AL CU SI:VA:
C14_LAVES :AL CU:AL CU:
DIAMOND_A4 :AL SI:
C15_LAVES :AL CU SI:AL CU SI:
C36_LAVES :AL CU:AL CU:
AL2CU_C16 :AL:AL CU SI:
ALCU_DEL :AL:CU:
ALCU_EPS :AL CU:CU:
ALCU_ETA :AL CU:CU:
ALCU_PRIME :AL:CU:
ALCU_ZETA :AL:CU:
GAMMA_D83 :AL SI:AL CU SI:CU:
GAMMA_H :AL:AL CU:CU:
CU15SI4_EPSILON :CU:AL SI:
CU33SI7_DELTA :CU:SI:
CU56SI11_GAMMA :CU SI:SI:
CUSI_ETA :CU:SI:
TDB_ALDEMO: get
... the command in full is GET_DATA
REINITIATING GES5 .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ...

List of references for assessed data

'A. Dinsdale, Calphad, 15 (1991) 317-425; unary data'
'Volume data from TCFE4, 2006'
'X.-G. Lu, et al., CALPHAD, 29 (2005) 68-89; Molar volumes'
'X.-G. Lu, Thermo-Calc Software AB, 2006; Molar volumes'
'I. Ansara (Editor), COST 507, (1998)'
'X.Y. Yan, J. Alloy and Compd. 308, 221-229 (2000), Cu-Si'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
'J. Groebner, Calphad, 20(2) 247-254 (1996), Al-C-Si'
'C.-Y. He, Calphad, 33, 200-210 (2009), Al-Cu-Si'
'Volume data, N. Dupin 2008'
'L. Kjellqvist, Thermo-Calc Software AB, 2010; Unassessed parameter,
linear combination of unary volume data'
'Hai-Lin Chen, in TCAL2.0, Extrapolations, assumptions
adjustment'
'J.R.Zhao, Y.Du, in , 2010, Sn-Sr, Cu-Mg-Si'
'L. Kjellqvist, Thermo-Calc Software AB, 2012; Molar volumes'
'W.H. Sun, unpublished (2010), Cu-Si-Zn, Cu-Ni-Zn'
-OK-
TDB_ALDEMO: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3: @@ The composition
POLY_3: s-c w(si)=.09,w(cu)=.10,t=1000,p=1e5,n=1
... the command in full is SET_CONDITION
POLY_3: l-c
... the command in full is LIST_CONDITIONS
W(SI)=9E-2, W(CU)=0.1, T=1000, P=1E5, N=1
DEGREES OF FREEDOM 0
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 16528 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY_3: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
Output from POLY-3, equilibrium = 1, label A0 , database: ALDEMO

Conditions:
W(SI)=9E-2, W(CU)=0.1, T=1000, P=1E5, N=1
DEGREES OF FREEDOM 0
```



```

Temperature 1000.00 K ( 726.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 2.87371E+01
Total Gibbs energy -4.64558E+04, Enthalpy 3.21074E+04, Volume 1.02742E-05

Component      Moles      W-Fraction  Activity  Potential  Ref.stat
AL              8.6269E-01  8.1000E-01  5.0275E-03 -4.4007E+04 SER
CU              4.5223E-02  1.0000E-01  3.2656E-06 -1.0503E+05 SER
SI              9.2090E-02  9.0000E-02  7.5475E-03 -4.0629E+04 SER

LIQUID          Status ENTERED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 2.8737E+01, Volume fraction 1.0000E+00 Mass fractions:
AL 8.10000E-01 CU 1.00000E-01 SI 9.00000E-02
POLY_3:Hit RETURN to continue
POLY_3: @@ Set temperature as axis
POLY_3: s-a-v
... the command in full is SET_AXIS_VARIABLE
Axis number: /1/: 1
Condition /NONE/: t
Min value /0/: 500
Max value /1/: 1000
Increment /12.5/: 12.5
POLY_3: save tcex14 y
... the command in full is SAVE_WORKSPACES
POLY_3: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 1000.000
...OK

Phase Region from 1000.000 for:
LIQUID
Global test at 9.20000E+02 .... OK
Global check of adding phase at 8.42133E+02
Calculated 18 equilibria

Phase Region from 842.133 for:
FCC_L12
LIQUID
Global check of adding phase at 8.28227E+02
Calculated 5 equilibria

Phase Region from 828.227 for:
DIAMOND_A4
FCC_L12
LIQUID
Global check of adding phase at 7.94999E+02
Calculated 6 equilibria

Phase Region from 794.999 for:
AL2CU_C16
DIAMOND_A4
FCC_L12
LIQUID
Calculated 2 equilibria

Phase Region from 794.999 for:
AL2CU_C16
DIAMOND_A4
FCC_L12
Global test at 7.20000E+02 .... OK
Global test at 6.20000E+02 .... OK
Global test at 5.20000E+02 .... OK
Terminating at 500.000
Calculated 33 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex14\tcex
14.POLY3
POLY_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

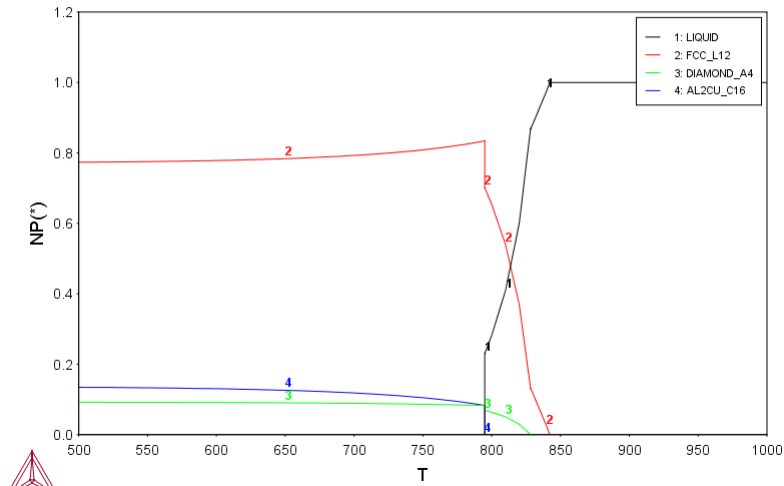
Setting automatic diagram axes

POST: @@ Plot phase fractions
POST: S-D-A X T
... the command in full is SET_DIAGRAM_AXIS
POST: S-D-A Y NP(*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: S-LAB D
... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: set-title example 14a
POST: plot
... the command in full is PLOT_DIAGRAM

```

# example 14a

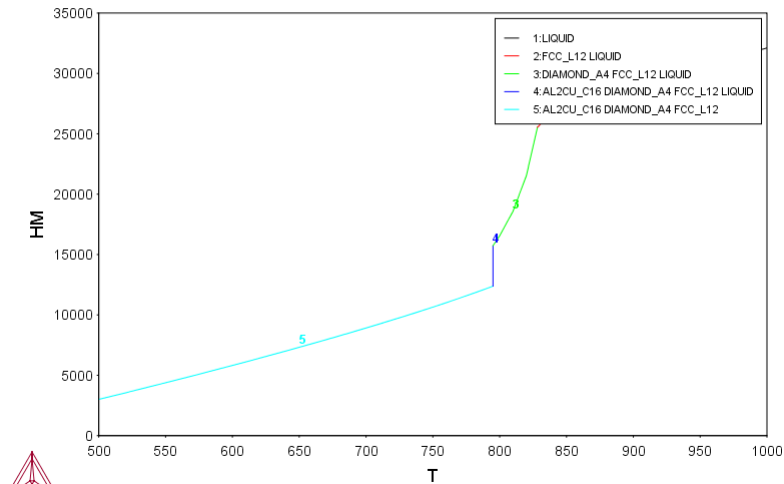
2016.05.16.13.29.12  
ALDEMO: AL, CU, SI  
W(SI)=9E-2, W(CU)=0.1, P=1E5, N=1.



POST:  
POST:Hit RETURN to continue  
POST: @@ Plot the total enthalpy (heat)  
POST: S-D-A Y HM  
... the command in full is SET\_DIAGRAM\_AXIS  
POST: S-LAB B  
... the command in full is SET\_LABEL\_CURVE\_OPTION  
POST: set-title example 14b  
POST:  
POST: plot  
... the command in full is PLOT DIAGRAM

# example 14b

2016.05.16.13.29.12  
ALDEMO: AL, CU, SI  
W(SI)=9E-2, W(CU)=0.1, P=1E5, N=1.



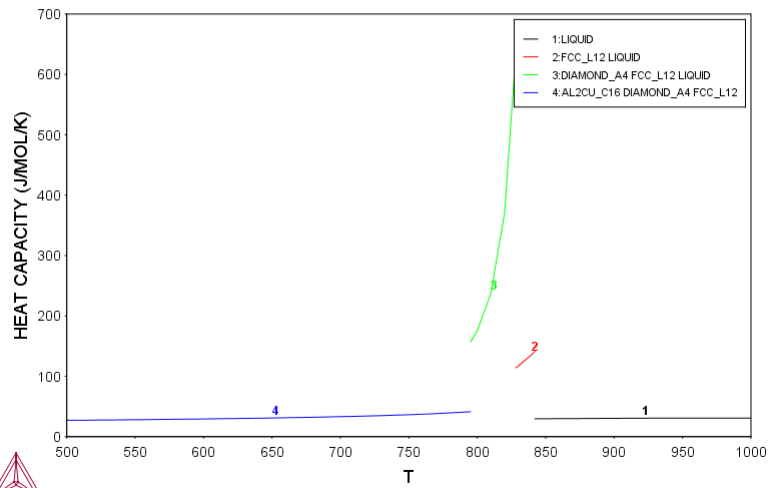
POST:  
POST:Hit RETURN to continue  
POST: @@ Plot the heat capacity. This must first be entered as  
POST: @@ a function as derivatives cannot be plotted directly.  
POST: ENT FUN CP=HM.T;  
... the command in full is ENTER\_SYMBOL  
POST: S-D-A Y CP  
... the command in full is SET\_DIAGRAM\_AXIS  
POST: S-S  
... the command in full is SET\_SCALING\_STATUS  
AXIS (X, Y OR Z) : Y  
AUTOMATIC SCALING (Y OR N) /N/: N  
MIN VALUE : 0  
MAX VALUE : 700  
POST: S-A-T-S  
... the command in full is SET\_AXIS\_TEXT\_STATUS  
AXIS (X, Y OR Z) : Y  
AUTOMATIC AXIS TEXT (Y OR N) /N/: N  
AXIS TEXT : HEAT CAPACITY (J/MOL/K)  
POST: set-title example 14c  
POST:  
POST: plot  
... the command in full is PLOT DIAGRAM

### example 14c

2016.05.16 13:29:13

ALDEMO: AL, CU, SI

W(SI)=9E-2, W(CU)=0.1, P=1E5, N=1.



POST:

POST: set-inter

... the command in full is SET\_INTERACTIVE\_MODE

POST:

About Linked: Mon May 16 09:31:44 2016

```

SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex15\tcex15.TCM"SYS: SET_ECHO
SYS: @@
SYS: @@
SYS: @@ This is an example of a solidification simulation of a Cr-Ni alloy.
SYS: @@ No back diffusion in the solid, i.e. Scheil-Gulliver model.
SYS: @@
SYS: SET-LOG ex15,,,
SYS: GO SCHEIL
... the command in full is GOTO_MODULE
SCHEIL: TEMPERATURE-STEP
Temperature step (C) /1/: 5
SCHEIL: START-WIZARD
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
L12_FCC          B2_BCC          B2_VACANCY
HIGH_SIGMA       DICTRA_FCC_A1   REJECTED
Database /TCFE8/: TCFE7
Current database: Steels/Fe-Alloys v7.0

VA DEFINED
L12_FCC          B2_BCC          B2_VACANCY
HIGH_SIGMA       DICTRA_FCC_A1   REJECTED
Major element or alloy: cr
Composition input in mass (weight) percent? /Y/: n
Composition will be taken to be in mole percent
1st alloying element: ni
Mole percent /1/: 10
2nd alloying element:
Temperature (C) /2000/: 2000
VA DEFINED
L12_FCC          B2_BCC          B2_VACANCY
HIGH_SIGMA       DICTRA_FCC_A1   REJECTED
REINITIATING GES5 .....
... the command in full is DEFINE_ELEMENTS
CR DEFINED
... the command in full is DEFINE_ELEMENTS
NI DEFINED

This database has following phases for the defined system

LIQUID:L          BCC_A2          FCC_A1
HCP_A3            SIGMA           CHI_A12
LAVES_PHASE_C14   CR3SI          NBNi3
NI3TI

Reject phase(s) /NONE/: *
LIQUID:L          BCC_A2          FCC_A1
HCP_A3            SIGMA           CHI_A12
LAVES_PHASE_C14   CR3SI          NBNi3
NI3TI_REJECTED
Restore phase(s):: liq bcc fcc
LIQUID:L          BCC_A2          FCC_A1
RESTORED
Restore phase(s): /NONE/: NONE

.....

The following phases are retained in this system:

LIQUID:L          BCC_A2          FCC_A1
.....

OK? /Y/: y
GAS:G REJECTED
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
'J. Brillo and I. Egry, Int. J. Thermophysics, 24, pp. 1155-1170'
'J. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR-NI'
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
Molar volumes'
'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
-OK-
Should any phase have a miscibility gap check? /N/:
LIQUID PHASE NAME: LIQUID
Fast diffusing components: /NONE/:
... the command in full is SET_NUMERICAL_LIMITS
... the command in full is COMPUTE_TRANSITION
This command is a combination of CHANGE_STATUS and SET_CONDITION
to calculate directly when a phase may form by releasing one condition.
You must release one of these conditions
T=2273.15, X(NI)=0.1, P=1E5, N=1 DEGREES OF FREEDOM 0
To form BCC_A2#1 the condition is set to T=2058.59460117
CALCULATING USING NORMAL EQUILIBRIUM CONDITIONS
... the command in full is ADD_INITIAL_EQUILIBRIUM
... the command in full is ADVANCED_OPTIONS
... the command in full is STEP_WITH_OPTIONS
...OK

Phase Region from 2058.58 for:
LIQUID
BCC_A2
Global Check of removing phase at 2.05859E+03
Calculated 3 equilibria

```

```

Phase Region from 2058.59 for:
LIQUID
Terminating at 2058.68
Calculated 4 equilibria

Phase Region from 2058.58 for:
LIQUID
BCC_A2
Global test at 2.01858E+03 .... OK
Global test at 1.96858E+03 .... OK
Global test at 1.91858E+03 .... OK
Global check of removing phase at 1.89734E+03
Calculated 35 equilibria

Phase Region from 1897.34 for:
BCC_A2
Calculated 4 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex15\SCHE
IL_4176.POLY3

POSTPROCESSOR VERSION 3.2

```

Setting automatic diagram axes

POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

```

... the command in full is ENTER_SYMBOL
... the command in full is MAKE_EXPERIMENTAL_DATAFI
An EXP file c:\jenkins\WORKSP~1\THERMO~1\examples\tcex15\SCHEIL_EQ_4176.EXP
has been created to store the equilibrium solidification results.
... the command in full is READ_WORKSPACES
CALCULATING SCHEIL SOLIDIFICATION
... the command in full is SET_NUMERICAL_LIMITS

```

```

T(C)      fraction solid

1785.535   0.000000

```

PHASE REGION:LIQUID + BCC\_A2

```

T(C)      fraction solid

1785.378   0.8823747E-03
1780.378   0.6490648E-01
1775.378   0.1226306
1770.378   0.1748823
1765.378   0.2223552
1760.378   0.2656343
1755.378   0.3052160
1750.378   0.3415242
1745.378   0.3749225
1740.378   0.4057245
1735.378   0.4342018
1730.378   0.4605909
1725.378   0.4850982
1720.378   0.5079050
1715.378   0.5291708
1710.378   0.5490363
1705.378   0.5676264
1700.378   0.5850522
1695.378   0.6014127
1690.378   0.6167963
1685.378   0.6312824
1680.378   0.6449423
1675.378   0.6578403
1670.378   0.6700345
1665.378   0.6815775
1660.378   0.6925168
1655.378   0.7028958
1650.378   0.7127541
1645.378   0.7221276
1640.378   0.7310493
1635.378   0.7395494
1630.378   0.7476556
1625.378   0.7553933
1620.378   0.7627859
1615.378   0.7698550
1610.378   0.7766207
1605.378   0.7831013
1600.378   0.7893139
1595.378   0.7952744
1590.378   0.8009975
1585.378   0.8064969
1580.378   0.8117854
1575.378   0.8168749
1570.378   0.8217764
1565.378   0.8265005
1560.378   0.8310568
1555.378   0.8354544
1550.378   0.8397021
1545.378   0.8438078
1540.378   0.8477792
1535.378   0.8516235
1530.378   0.8553475
1525.378   0.8589580
1520.378   0.8624606
1515.378   0.8658613
1510.378   0.8691657
1505.378   0.8723790
1500.378   0.8755064
1495.378   0.8785528
1490.378   0.8815228
1485.378   0.8844210
1480.378   0.8872519
1475.378   0.8900197
1470.378   0.8927287
1465.378   0.8953829
1460.378   0.8979866
1455.378   0.9005436

```

1450.378	0.9030572
1445.378	0.9055331
1440.378	0.9079746
1435.378	0.9103858
1430.378	0.9127710
1425.378	0.9151344
1420.378	0.9174805
1415.378	0.9198139
1410.378	0.9221392
1405.378	0.9244614
1400.378	0.9267856
1395.378	0.9291170
1390.378	0.9314612
1385.378	0.9338239
1380.378	0.9362111
1375.378	0.9386289
1370.378	0.9410835
1365.378	0.9435813
1360.378	0.9461287
1355.378	0.9487319
1350.378	0.9513970
1345.378	0.9541295
1344.910	0.9543771

PHASE REGION:BCC\_A2 + FCC\_A1

T(C)            fraction solid

1344.753        1.0000000

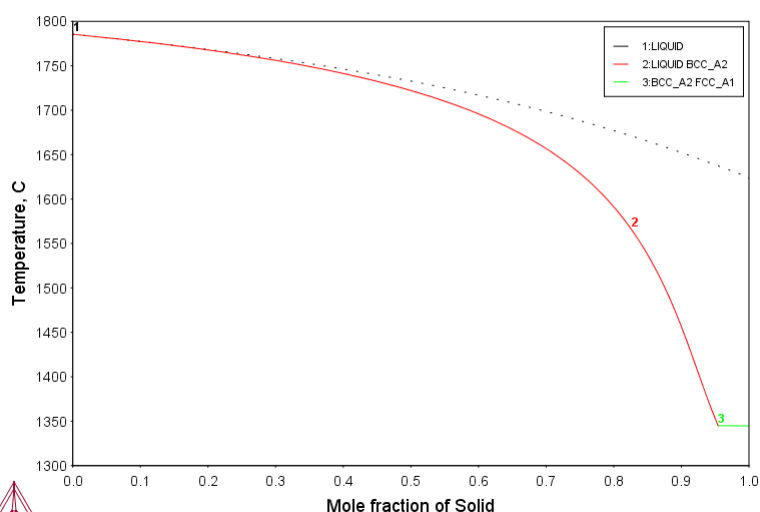
Hint: move the last function to the first equilibrium where it is used

... the command in full is SET\_LABEL\_CURVE\_OPTION  
 ... the command in full is APPEND EXPERIMENTAL DATA

2016.05.16.13.31.21

TCFE7: CR, NI

T=2058.68, X(NI)=0.1, P=1E5, N=1



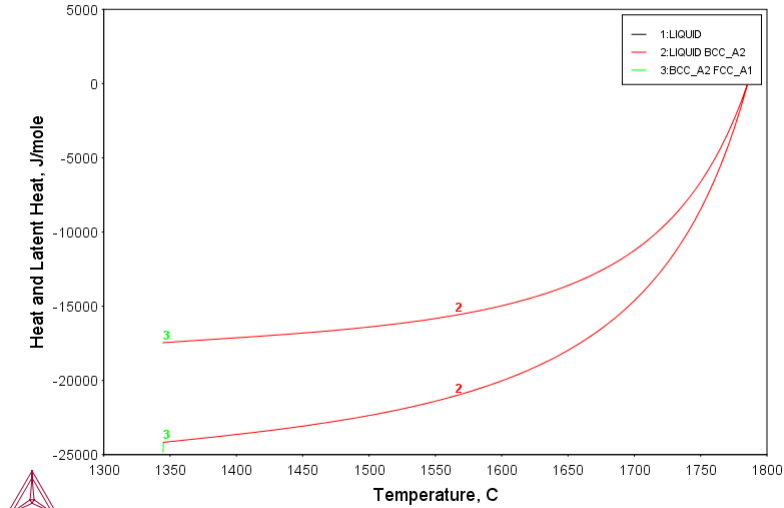
... the command in full is APPEND\_EXPERIMENTAL\_DATA

The following axis variables are available

T --- Temperature in Celsius  
 NL/BL --- Mole/mass fraction of liquid  
 NS/BS --- Mole/mass fraction of all solid phases  
 NS(ph)/BS(ph) --- Mole/mass fraction of a solid phase  
 W(ph,el) --- Weight fraction of an element in a phase  
 X(ph,el) --- Mole fraction of an element in a phase  
 Y(ph,el) --- Site fraction of an element in a phase  
 NN(ph,el) --- Distribution of an element in a phases  
 NH/BH --- Heat release and Latent heat per mole/gram  
 CP/BCP --- Apparent heat capacity per mole/gram  
 NV/NV(ph) --- Molar volume of the system or a phase  
 DS/DS(ph) --- Average density of the system or a phase  
 BT --- Apparent volumetric TEC of the system

"el" and "ph" are name of element and phase, respectively  
 "\*" can be used as a wild character for "el" and "ph"

POST: s-d-a x t  
 ... the command in full is SET\_DIAGRAM\_AXIS  
 POST: s-d-a y nh  
 ... the command in full is SET\_DIAGRAM\_AXIS  
 POST: plot,/////////  
 ... the command in full is PLOT\_DIAGRAM



POST: set-inter  
... the command in full is SET\_INTERACTIVE\_MODE  
POST:

## tcex16

**About** simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software (build 9533) running on WinNT 64-bit wordlength  
Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118  
License library version: 8.5.1.0017  
Linked: Mon May 16 09:31:44 2016

```
SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex16\tcex16.TCM" set-echo
```

```
SYS: @@
```

```
SYS: @@
```

```
SYS: @@ Calculation of the second order transition line in the Bcc field of the Al-Fe system
```

```
SYS: @@
```

```
SYS: SET-LOG ex16,,
```

```
SYS: GO DA
```

```
... the command in full is GOTO_MODULE
```

```
THERMODYNAMIC DATABASE module
```

```
Current database: Steels/Fe-Alloys v8.0
```

```
VA DEFINED
```

```
L12_FCC
```

```
B2_BCC
```

```
B2_VACANCY
```

```
HIGH_SIGMA
```

```
DICTRA_FCC_A1 REJECTED
```

```
TDB_TCFE8: SW SSOL5
```

```
... the command in full is SWITCH_DATABASE
```

```
Current database: SGTE Alloy Solutions Database v5.0
```

```
VA DEFINED
```

```
GAS:G REJECTED
```

```
TDB_SSOL5: D-SYS AL FE
```

```
... the command in full is DEFINE_SYSTEM
```

```
AL
```

```
FE DEFINED
```

```
TDB_SSOL5: REJ PH /ALL
```

```
... the command in full is REJECT
```

```
LIQUID:L
```

```
FCC_A1
```

```
FCC_L12
```

```
BCC_A2
```

```
BCC_B2
```

```
B2_BCC
```

```
HCP_A3
```

```
HCP_ZN
```

```
DHCP
```

```
DIAMOND_A4
```

```
BCT_A5
```

```
TETRAGONAL_U
```

```
CBCC_A12
```

```
CUB_A13
```

```
ORTHORHOMBIC_A20
```

```
RHOMBO_C19
```

```
LAVES_C14
```

```
LAVES_C15
```

```
LAVES_C36
```

```
M4N
```

```
ALM_D019
```

```
ALCE_AMORPHOUS
```

```
ALCU_THETA
```

```
AL2FE
```

```
AL5FE2
```

```
AL5FE4
```

```
AL13FE4
```

```
ALLI
```

```
AL4MN
```

```
AL6MN
```

```
AL11MN4
```

```
AL12MN
```

```
ALNB3
```

```
AL3NB
```

```
AL3NI2
```

```
ALPT3
```

```
ALTI
```

```
CR3SI_A15
```

```
D_GAMMA
```

```
FEPD
```

```
FEPD3
```

```
FESB
```

```
FEU6
```

```
FE2U
```

```
FEZN_GAMMA_D82
```

```
FEZN4
```

```
FEZN_DELTA
```

```
FEZN_ZETA
```

```
FEUZR_DELTA
```

```
FEZR2
```

```
FEZR3
```

```
REJECTED
```

```
TDB_SSOL5: @@ The BCC phase has B2 ordering in this system
```

```
TDB_SSOL5: @@ Note that this is modelled with two sublattices
```

```
TDB_SSOL5: @@ with both components in both sublattices
```

```
TDB_SSOL5: REST PH LIQ BCC_B2 BCC_A2
```

```
... the command in full is RESTORE
```

```
LIQUID:L
```

```
BCC_B2
```

```
BCC_A2
```

```
RESTORED
```

```
TDB_SSOL5: LI-SYS
```

```
... the command in full is LIST_SYSTEM
```

```
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:
```

```
LIQUID:L :AL FE:
```

```
BCC_A2 :AL FE:VA:
```

```
BCC_B2 :AL FE:AL FE:VA:
```

```
TDB_SSOL5: GET
```

```
... the command in full is GET_DATA
```

```
REINITIATING GES5 .....
```

```
ELEMENTS .....
```

```
SPECIES .....
```

```
PHASES .....
```

```
... the command in full is AMEND_PHASE_DESCRIPTION
```

```
... the command in full is AMEND_PHASE_DESCRIPTION
```

```
... the command in full is AMEND_PHASE_DESCRIPTION
```

```
PARAMETERS ...
```

```
FUNCTIONS ....
```

```
List of references for assessed data
```

```
'Data for the Al-Fe system were from an unpublished assessment of M  
Seiersten published in the COST507 final report: COST507  
Thermochemical Database for Light Metal Alloys, Vol 2, eds by I Ansara,  
AT Dinsdale and MH Rand, July 1998, EUR18499. >> Al-Fe '
```

```
-OK-
```

```
TDB_SSOL5: GO P-3
```

```
... the command in full is GOTO_MODULE
```

```
POLY version 3.32
```

```
POLY_3:
```

```
POLY_3: advanced global_minimization y 10000
```

```
... the command in full is ADVANCED_OPTIONS
```

```
Settings for global minimization:
```

```
POLY_3:
```

```
POLY_3: @@ Set conditions where the BCC phase should be ordered
```

```
POLY_3: SET-COND P=1E5,N=1,T=400,X(AL)=.4
```

```
... the command in full is SET_CONDITION
```

```
POLY_3: COMP-EQ
```

```
... the command in full is COMPUTE_EQUILIBRIUM
```

```
Using global minimization procedure
```

```
Calculated 10065 grid points in 0 s
```

```
Found the set of lowest grid points in 0 s
```

```
Calculated POLY solution 0 s, total time 0 s
```

```
POLY_3: @@ Use option N in order to see how Al and Fe distribute
```

```
POLY_3: @@ on the sublattices
```

```
POLY_3: LIST-EQ
```

```
... the command in full is LIST_EQUILIBRIUM
```

```
OUTPUT TO SCREEN OR FILE /SCREEN/:
```

```
Options /VWCS/: N
```

```
Output from POLY-3, equilibrium = 1, label A0 , database: SSOL5
```



```

Conditions:
P=1E5, N=1, T=400, X(AL)=0.4
DEGREES OF FREEDOM 0

Temperature 400.00 K ( 126.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 4.43010E+01
Total Gibbs energy -3.81486E+04, Enthalpy -2.55850E+04, Volume 0.00000E+00

Component      Moles      W-Fraction  Activity   Potential  Ref.stat
AL              4.0000E-01  2.4362E-01  4.1973E-08 -5.6493E+04 SER
FE              6.0000E-01  7.5638E-01  4.1248E-04 -2.5919E+04 SER

BCC_B2          ORD      Status ENTERED   Driving force 0.0000E+00
Moles 1.0000E+00, Mass 4.4301E+01, Volume fraction 0.0000E+00 Mass fractions:
FE 7.56376E-01 AL 2.43624E-01
Constitution:
Sublattice 1, Number of sites 5.0000E-01
FE 9.99996E-01 AL 4.22881E-06
Sublattice 2, Number of sites 5.0000E-01
AL 7.99996E-01 FE 2.00004E-01
Sublattice 3, Number of sites 3.0000E+00
VA 1.00000E+00
POLY_3:Hit RETURN to continue
POLY_3: @@ Change the condition of Al amount to be that the site-fractions
POLY_3: @@ in the two sublattices will have a certain difference. If they
POLY_3: @@ are the same the BCC phase is disordered
POLY_3: SET-COND X(AL)=NONE
... the command in full is SET_CONDITION
POLY_3: SET-COND Y(BCC_B2,FE#1)-Y(BCC_B2,FE#2)=0.1
... the command in full is SET_CONDITION
POLY_3: COMP-EQ
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Using already calculated grid
26 ITS, CPU TIME USED 0 SECONDS
POLY_3: LIST-EQ
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWNS/:Hit RETURN to continue
Options /VWNS/: @@ Set the difference smaller. This is as close to the second order
Output from POLY-3, equilibrium = 1, label A0 , database: SSOL5

Conditions:
P=1E5, N=1, T=400, Y(BCC_B2,FE)-Y(BCC_B2,FE#2)=0.1
DEGREES OF FREEDOM 0

Temperature 400.00 K ( 126.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 5.36842E+01
Total Gibbs energy -1.86969E+04, Enthalpy -4.69474E+03, Volume 0.00000E+00

Component      Moles      W-Fraction  Activity   Potential  Ref.stat
AL              7.4926E-02  3.7658E-02  7.3790E-14 -1.0056E+05 SER
FE              9.2507E-01  9.6234E-01  2.6569E-02 -1.2066E+04 SER

BCC_B2          ORD      Status ENTERED   Driving force 0.0000E+00
Moles 1.0000E+00, Mass 5.3684E+01, Volume fraction 0.0000E+00 Mass fractions:
FE 9.62342E-01 AL 3.76585E-02
Constitution:
Sublattice 1, Number of sites 5.0000E-01
FE 9.75074E-01 AL 2.49265E-02
Sublattice 2, Number of sites 5.0000E-01
FE 8.75074E-01 AL 1.24926E-01
Sublattice 3, Number of sites 3.0000E+00
VA 1.00000E+00
POLY_3: @@ transition as it is possible to be
POLY_3: SET-COND Y(BCC_B2,FE#1)-Y(BCC_B2,FE#2)=1E-4
... the command in full is SET_CONDITION
POLY_3: COMP-EQ
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Using already calculated grid
14 ITS, CPU TIME USED 0 SECONDS
POLY_3: @@ Now vary the temperature using these conditions
POLY_3: SET-AXIS-VAR 1
... the command in full is SET_AXIS_VARIABLE
Condition /NONE/: T
Min value /0/: 400
Max value /1/: 2000
Increment /40/: 10
POLY_3: @@ Always save before STEP or MAP (unless you want to overlay the new
POLY_3: @@ results on some previous results)
POLY_3: SAVE tcex16 Y
... the command in full is SAVE_WORKSPACES
POLY_3: STEP NORMAL
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 400.000
...OK

Phase Region from 400.000 for:
BCC_B2
Global test at 4.80000E+02 .... OK
Global test at 5.80000E+02 .... OK
Global test at 6.80000E+02 .... OK
Global test at 7.80000E+02 .... OK
Global test at 8.80000E+02 .... OK
Global test at 9.80000E+02 .... OK
Global test at 1.08000E+03 .... OK
Global test at 1.18000E+03 .... OK
Global test at 1.28000E+03 .... OK
Global test at 1.38000E+03 .... OK
Global test at 1.48000E+03 .... OK
Global test at 1.58000E+03 .... OK
Global check of adding phase at 1.64515E+03
Calculated 127 equilibria

Phase Region from 1645.15 for:
LIQUID
BCC_B2
Global check of removing phase at 1.64515E+03
Calculated 3 equilibria

```

Phase Region from 1645.15 for:  
 BCC\_B2  
 Global check of adding phase at 1.64515E+03  
 Calculated 3 equilibria

Phase Region from 1645.15 for:  
 LIQUID  
 BCC\_B2  
 Calculated 3 equilibria  
 Sorry cannot continue 0 189 1 1.6451539E+03  
 \*\*\* Buffer saved on file:  
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex16\tcex  
 16.POLY3

POLY\_3: POST

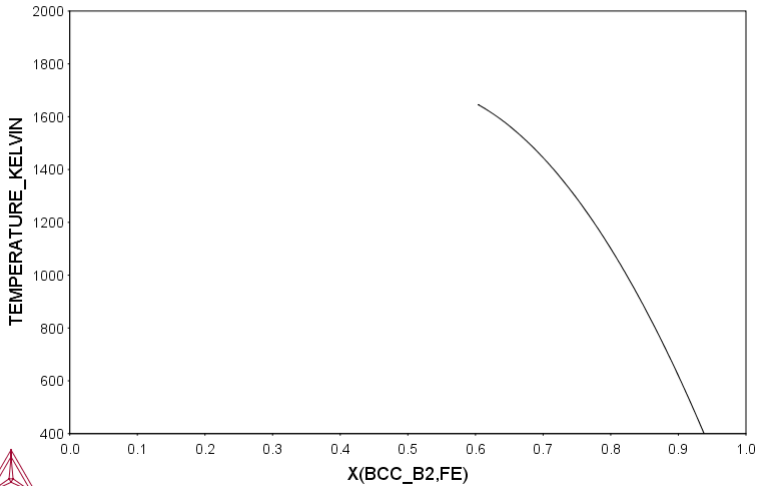
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: SET-DIA-AXIS X X(BCC\_B2,FE)  
 ... the command in full is SET\_DIAGRAM\_AXIS  
 POST: SET-DIA-AXIS Y T-K  
 ... the command in full is SET\_DIAGRAM\_AXIS  
 POST: SET-SCAL X N 0 1  
 ... the command in full is SET\_SCALING\_STATUS  
 POST: SET-SCAL Y N 400 2000  
 ... the command in full is SET\_SCALING\_STATUS  
 POST:  
 POST: set-title example 16a  
 POST: PLOT  
 ... the command in full is PLOT DIAGRAM

example 16a

2016.05.16.13.33.36  
 SSOL5:AL,FE  
 P=1E5,N=1,Y(BCC\_B2,FE)-Y(BCC\_B2,FE#2)=1.00017E-4



POST:  
 POST:Hit RETURN to continue  
 POST: @@ Write on file for plotting together with phase diagram  
 POST: MAKE TCX16  
 ... the command in full is MAKE\_EXPERIMENTAL\_DATAFI  
 POST: Y  
 No such command, use HELP  
 POST: BACK  
 POLY\_3: GO DA  
 ... the command in full is GOTO\_MODULE  
 TDB\_SSOL5: @@ Get data for all phases stable in Al-Fe  
 TDB\_SSOL5: REJ-SYS  
 ... the command in full is REJECT  
 VA DEFINED  
 GAS:G REJECTED  
 REINITIATING GES5 .....

TDB\_SSOL5: D-SYS AL FE  
 ... the command in full is DEFINE\_SYSTEM  
 AL FE DEFINED

TDB\_SSOL5: L-SYS  
 ... the command in full is LIST\_SYSTEM

ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENTS/: CONSTITUENT

LIQUID:L	:AL FE:
FCC_A1	:AL FE:VA:
FCC_L12	:AL FE:AL FE:VA:
BCC_A2	:AL FE:VA:
BCC_B2	:AL FE:AL FE:VA:
B2_BCC	:AL:VA:
HCP_A3	:AL FE:VA:
HCP_ZN	:AL:VA:
DHCP	:AL:
DIAMOND_A4	:AL:
BCT_A5	:AL:
TETRAGONAL_U	:FE:
CBCC_A12	:AL FE:VA:
CUB_A13	:AL FE:VA:
ORTHORHOMBIC_A20	:FE:
RHOMBO_C19	:AL:
LAVES_C14	:AL FE:AL FE:
LAVES_C15	:AL FE:AL FE:
LAVES_C36	:AL:AL:
M4N	:FE:VA:
ALM_D019	:AL:AL:
ALCE_AMORPHOUS	:AL:
ALCU_THETA	:AL:AL:
AL2FE	:AL:FE:
AL5FE2	:AL:FE:
AL5FE4	:AL FE:
AL13FE4	:AL:FE:AL VA:

```

ALLI      :AL:VA:
AL4MN     :AL:FE:
AL6MN     :AL:FE:
AL11MN4   :AL:FE:
AL12MN    :AL:FE:
ALNB3     :AL:AL:
AL3NB     :AL:AL:
AL3NI2    :AL:AL:VA:
ALPT3     :AL:AL:
ALTI      :AL:AL:
CR3SI_A15 :FE:AL:VA:
D_GAMMA   :AL:
FEPD      :FE:FE:
FEPD3     :FE:FE:
FESB      :FE:FE:
FEU6      :FE:FE:
FE2U      :FE:FE:
FEZN_GAMMA_D82 :FE:FE:
FEZN4     :FE:FE:
FEZN_DELTA :FE:FE:
FEZN_ZETA :FE:FE:
FEUZR_DELTA :FE:FE:
FEZR2     :FE:FE:
FEZR3     :FE:FE:
TDB_SSOL5: REJ PH /ALL
... the command in full is REJECT
LIQUID:L      FCC_A1      FCC_L12
BCC_A2        BCC_B2      B2_BCC
HCP_A3        HCP_ZN      DHCP
DIAMOND_A4    BCT_A5      TETRAGONAL_U
CBCC_A12      CUB_A13     ORTHORHOMBIC_A20
RHOMBO_C19    LAVES_C14   LAVES_C15
LAVES_C36     M4N         ALM_D019
ALCE_AMORPHOUS ALCU_THETA AL2FE
AL5FE2        AL5FE4      AL13FE4
ALLI          AL4MN       AL6MN
AL11MN4       AL12MN      ALNB3
AL3NB         AL3NI2      ALPT3
ALTI          CR3SI_A15   D_GAMMA
FEPD          FEPD3       FESB
FEU6          FE2U        FEZN_GAMMA_D82
FEZN4         FEZN_DELTA  FEZN_ZETA
FEUZR_DELTA   FEZR2       FEZR3
REJECTED
TDB_SSOL5: REST PH LIQ BCC_B2 FCC_A1 BCC_A2 AL13FE4 AL2FE AL5FE2 AL5FE4
... the command in full is RESTORE
LIQUID:L      BCC_B2      FCC_A1
BCC_A2        AL13FE4     AL2FE
AL5FE2        AL5FE4      RESTORED
TDB_SSOL5: GET
... the command in full is GET_DATA
REINITIATING GES5 .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

'Data for the Al-Fe system were from an unpublished assessment of M
Seiersten published in the COST507 final report: COST507
Thermochemical Database for Light Metal Alloys, Vol 2, eds by I Ansara,
AT Dinsdale and MH Rand, July 1998, EUR18499. >> Al-Fe '
-OK-
TDB_SSOL5: GO P-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3: @@ Calculate an equilibrium where BCC is ordered
POLY_3: S-C T=1300,P=1E5,N=1,X(AL)=.3
... the command in full is SET_CONDITION
POLY_3: C-E
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 10478 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY_3: @@ List the equilibrium. Note that option N gives the
POLY_3: @@ constitution of the BCC phase and this shows that the
POLY_3: @@ site-fractions are different in the two sublattices,
POLY_3: @@ i.e. the BCC is ordered
POLY_3: L-E
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWNS/: N
Output from POLY-3, equilibrium = 1, label A0 , database: SSOL5

Conditions:
T=1300, P=1E5, N=1, X(AL)=0.3
DEGREES OF FREEDOM 0

Temperature 1300.00 K ( 1026.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 4.71875E+01
Total Gibbs energy -8.63003E+04, Enthalpy 1.26381E+04, Volume 0.00000E+00

Component      Moles      W-Fraction Activity Potential Ref.stat
AL              3.0000E-01  1.7154E-01  3.1606E-05 -1.1200E+05 SER
FE              7.0000E-01  8.2846E-01  9.4427E-04 -7.5285E+04 SER

BCC_B2          ORD      Status ENTERED Driving force 0.0000E+00
Moles 1.0000E+00, Mass 4.7187E+01, Volume fraction 0.0000E+00 Mass fractions:
FE 8.28459E-01 AL 1.71541E-01
Constitution:
Sublattice 1, Number of sites 5.0000E-01
FE 8.77450E-01 AL 1.22550E-01
Sublattice 2, Number of sites 5.0000E-01
FE 5.22550E-01 AL 4.77450E-01
Sublattice 3, Number of sites 3.0000E+00
VA 1.00000E+00
POLY_3:Hit RETURN to continue

```

```

POLY_3: @@ Set axis
POLY_3: S-A-V 1 X(AL)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: 1
Increment /.025/: .025
POLY_3: S-A-V 2 T
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 500
Max value /1/: 2000
Increment /37.5/: 25
POLY_3: SAVE tcex16 Y
... the command in full is SAVE_WORKSPACES

```

This file contains results from a previous STEP or MAP command.  
The SAVE command will save the current status of the program but destroy  
the results from the previous STEP or MAP commands.

```

POLY_3: MAP
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

```

Organizing start points

Using ADDED start equilibria

```

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Trying global minimization! 1
Creating a new composition set BCC_B2#2
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22

Phase region boundary 1 at: 8.364E-03 1.237E+03
  BCC_B2
  ** FCC_A1
Calculated 19 equilibria

Phase region boundary 2 at: 8.364E-03 1.237E+03
  BCC_B2
  ** FCC_A1
Calculated 39 equilibria

Phase region boundary 3 at: 3.562E-01 1.702E+03
  ** LIQUID
  BCC_B2
Calculated 35 equilibria

Phase region boundary 4 at: 3.562E-01 1.702E+03
  ** LIQUID
  BCC_B2
Calculated. 16 equilibria
Calculated. 16 equilibria

Phase region boundary 5 at: 3.562E-01 1.702E+03
  ** LIQUID
  BCC_B2
Calculated. 17 equilibria

Phase region boundary 6 at: 5.550E-01 1.496E+03
  ** LIQUID
  ** AL5FE4
  BCC_B2
Calculated. 7 equilibria

Phase region boundary 7 at: 5.452E-01 1.496E+03
  ** AL5FE4
  BCC_B2#2
Calculated. 7 equilibria

Phase region boundary 8 at: 5.672E-01 1.368E+03
  ** AL2FE
  ** AL5FE4
  BCC_B2#2
Calculated. 36 equilibria
Terminating at axis limit.

Phase region boundary 10 at: 6.316E-01 1.368E+03
  ** AL2FE
  AL5FE4
Calculated. 4 equilibria

```

Phase region boundary 11 at: 6.502E-01 1.428E+03  
 \*\* AL2FE  
 \*\* AL5FE2  
 AL5FE4  
  
 Phase region boundary 12 at: 6.740E-01 1.428E+03  
 \*\* AL5FE2  
 AL5FE4  
 Calculated. 2 equilibria  
  
 Phase region boundary 13 at: 6.744E-01 1.430E+03  
 \*\* LIQUID  
 \*\* AL5FE2  
 AL5FE4  
  
 Phase region boundary 14 at: 6.593E-01 1.430E+03  
 \*\* LIQUID  
 AL5FE4  
 Calculated. 8 equilibria  
 Terminating at known equilibrium  
  
 Phase region boundary 15 at: 6.993E-01 1.430E+03  
 \*\* LIQUID  
 AL5FE2  
 Calculated. 12 equilibria  
  
 Phase region boundary 16 at: 7.362E-01 1.424E+03  
 \*\* LIQUID  
 \*\* AL13FE4  
 AL5FE2  
  
 Phase region boundary 17 at: 7.337E-01 1.424E+03  
 \*\* AL13FE4  
 AL5FE2  
 Calculated.. 38 equilibria  
 Terminating at axis limit.  
  
 Phase region boundary 18 at: 7.556E-01 1.424E+03  
 LIQUID  
 \*\* AL13FE4  
 Calculated. 24 equilibria  
  
 Phase region boundary 19 at: 8.723E-01 9.271E+02  
 LIQUID  
 \*\* AL13FE4  
 \*\* FCC\_A1  
  
 Phase region boundary 20 at: 9.955E-01 9.271E+02  
 LIQUID  
 \*\* FCC\_A1  
 Calculated 10 equilibria  
  
 Phase region boundary 21 at: 8.813E-01 9.271E+02  
 AL13FE4  
 \*\* FCC\_A1  
 Calculated.. 19 equilibria  
 Terminating at axis limit.  
  
 Phase region boundary 22 at: 6.905E-01 1.428E+03  
 AL2FE  
 \*\* AL5FE2  
 Calculated.. 39 equilibria  
 Terminating at axis limit.  
  
 Phase region boundary 23 at: 5.550E-01 1.496E+03  
 \*\* LIQUID  
 BCC\_B2#2  
 Calculated 50 equilibria  
  
 Phase region boundary 24 at: 5.820E-01 5.100E+02  
 \*\* AL2FE  
 BCC\_B2#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.  
  
 Phase region boundary 25 at: 5.820E-01 5.100E+02  
 \*\* AL2FE  
 BCC\_B2#2  
 Calculated. 36 equilibria  
 Terminating at known equilibrium  
  
 Phase region boundary 26 at: 8.824E-01 5.100E+02  
 \*\* AL13FE4  
 FCC\_A1  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.  
  
 Phase region boundary 27 at: 8.824E-01 5.100E+02  
 \*\* AL13FE4  
 FCC\_A1  
 Calculated. 18 equilibria  
 Terminating at known equilibrium  
  
 Phase region boundary 28 at: 8.824E-01 5.100E+02  
 \*\* AL13FE4  
 FCC\_A1  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.  
  
 Phase region boundary 29 at: 8.824E-01 5.100E+02  
 \*\* AL13FE4  
 FCC\_A1  
 Calculated. 18 equilibria  
 Terminating at known equilibrium  
  
 Phase region boundary 30 at: 8.722E-01 1.003E+03  
 LIQUID  
 \*\* AL13FE4  
 Calculated. 5 equilibria  
 Terminating at known equilibrium  
  
 Phase region boundary 31 at: 8.722E-01 1.003E+03

```

    LIQUID
    ** AL13FE4
    Calculated.                28 equilibria
    Terminating at known equilibrium

Phase region boundary 32 at: 1.805E-02 1.497E+03
    ** BCC_B2
    FCC_A1
    Calculated                32 equilibria

Phase region boundary 33 at: 1.805E-02 1.497E+03
    ** BCC_B2
    FCC_A1
    Calculated                35 equilibria

Phase region boundary 34 at: 1.032E-02 1.813E+03
    LIQUID
    ** BCC_B2
    Calculated                13 equilibria

Phase region boundary 35 at: 1.032E-02 1.813E+03
    LIQUID
    ** BCC_B2
    Calculated.                44 equilibria
    Calculated                44 equilibria

Phase region boundary 36 at: 1.032E-02 1.813E+03
    LIQUID
    ** BCC_B2
    Calculated.                47 equilibria
    Terminating at known equilibrium

Phase region boundary 37 at: 3.201E-01 1.728E+03
    LIQUID
    ** BCC_B2
    Calculated                34 equilibria

Phase region boundary 38 at: 3.201E-01 1.728E+03
    LIQUID
    ** BCC_B2
    Calculated.                19 equilibria
    Calculated                19 equilibria

Phase region boundary 39 at: 3.201E-01 1.728E+03
    LIQUID
    ** BCC_B2
    Calculated.                22 equilibria
    Terminating at known equilibrium

Phase region boundary 40 at: 6.421E-01 1.451E+03
    LIQUID
    ** AL5FE4
    Calculated.                7 equilibria
    Calculated                7 equilibria

Phase region boundary 41 at: 6.421E-01 1.451E+03
    LIQUID
    ** AL5FE4
    Calculated.                6 equilibria
    Terminating at known equilibrium

Phase region boundary 42 at: 6.421E-01 1.451E+03
    LIQUID
    ** AL5FE4
    Calculated.                3 equilibria
    Terminating at known equilibrium

Phase region boundary 43 at: 8.763E-01 9.396E+02
    LIQUID
    ** AL13FE4
    Calculated.                28 equilibria
    Terminating at known equilibrium

Phase region boundary 44 at: 8.763E-01 9.396E+02
    LIQUID
    ** AL13FE4
    Calculated.                2 equilibria
    Terminating at known equilibrium
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex16\tcex
16.POLY3
CPU time for mapping                7 seconds
POLY_3:
POLY_3: POST

POLY-3 POSTPROCESSOR VERSION 3.2

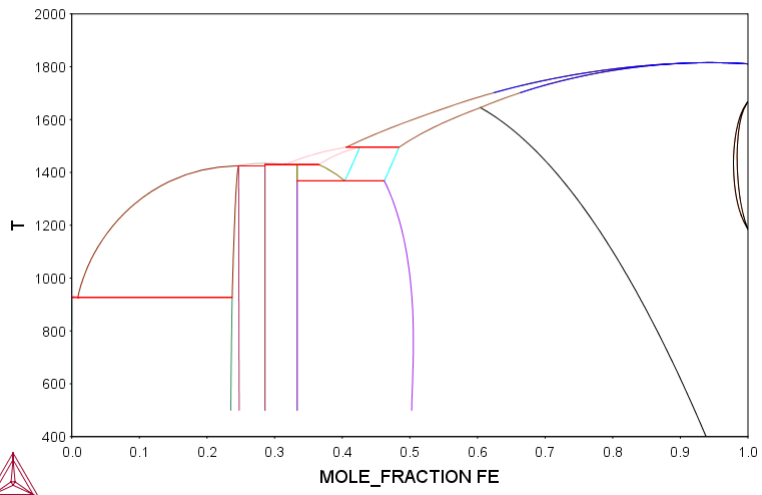
Setting automatic diagram axes

POST:
POST: S-D-A X M-F FE
... the command in full is SET_DIAGRAM_AXIS
POST: S-D-A Y T
... the command in full is SET_DIAGRAM_AXIS
POST: @@ Append the previous line for the 2nd order transition
POST: A-E-D Y TCX16
... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: set-title example 16b
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
The composition set BCC_B2#2 created from the store file

```

# example 16b

2016.05.16.13.33.50  
SSOL5: AL, FE  
P=1E5, N=1



POST:  
POST: set-inter  
... the command in full is SET\_INTERACTIVE\_MODE  
POST:

tcex17

About Software (build 9533) running on WinNT 64-bit wordlength  
Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118  
License library version: 8.5.1.0017  
Linked: Mon May 16 09:31:44 2016

SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex17\tcex17.TCM" set-echo

SYS: @@

SYS: @@

SYS: @@ Calculation of the pseudo-binary system CaO-SiO2

SYS: @@ using the ionic database

SYS: @@

SYS: set-log ex17,,,,

SYS: go da

... the command in full is GOTO\_MODULE

THERMODYNAMIC DATABASE module

Current database: Steels/Fe-Alloys v8.0

VA DEFINED

L12 FCC B2 BCC B2\_VACANCY

HIGH\_SIGMA DICTRA\_FCC\_A1 REJECTED

TDB\_TCFE8: @@ This database can be used both for pseudobinary systems like

TDB\_TCFE8: @@ the one in this case, CaO-SiO2, or for full ternary systems

TDB\_TCFE8: @@ like Ca-Fe-O.

TDB\_TCFE8: sw OXDEMO

... the command in full is SWITCH\_DATABASE

Current database: Oxide Demo Database

VA /- DEFINED

TDB\_OXDEMO: @@ Note that /- represent the 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 :CA CA101 CA2 O1SI1 O2 O2SI1 O2SI2 O3 SI SI2 SI3:

IONIC\_LIQ:Y :CA+2 SI+4:O-2 SIO4-4 VA SIO2:

> Ionic liquid mixture, modelled by the ionic two-sublattice model.

BCC A2 :CA SI:O VA:

CA2SIO4\_ALPHA :CA+2:SI+4:O-2:

> This is 2CaO.SiO2. Prototype Ca2[SiO4] (hP24, P63/mmc)

CA2SIO4\_ALPHA\_PRIME:I :CA+2:SI+4:O-2:

> This is 2CaO.SiO2. Prototype Sr2[SiO4] (oP52, Pnma)

CRISTOBALITE :SIO2:

> Prototype SiO2 (cF24, Fd3m)

DIAMOND\_FCC\_A4 :SI:O VA:

> Silicon (cF8, Fd-3m)

FCC A1 :CA SI:O VA:

HALITE:I :CA+2 VA:O-2:

> This is CaO and FeO (cI2, Im-3m)

HATRURITE :CA+2:SI+4:O-2:

> This is 3CaO.SiO2 (hR81, R3m)

HCP A3 :CA SI:VA:

LARNITE :CA+2:SI+4:O-2:

> This is 2CaO.SiO2 (metastable at 1 atm)

OLIVINE:I :CA+2:CA+2:SI+4:O-2:

> This is 2CaO.SiO2 and fayalite

PSEUDO\_WOLLASTONITE :CA+2:SI+4:O-2:

> This is CaO.SiO2 (mS120, C12/c1)

QUARTZ :SIO2:

> Prototype SiO2 (hP9, P3121 (rt) P6222 (ht))

RANKINITE :CA+2:SI+4:O-2:

> This is 3CaO.2SiO2 (mP48, P121/c1)

TRIDYMITE :SIO2:

> Prototype SiO2 (hP12, P63/mmc)

WOLLASTONITE:I :CA+2:SI+4:O-2:

> This is CaO.SiO2 (aP30, P-1)

TDB\_OXDEMO: @@ If we want to calculate a pseudobinary system

TDB\_OXDEMO: @@ we must take away all phases and constituents that make it

TDB\_OXDEMO: @@ possible for the phase to exist outside the composition line

TDB\_OXDEMO: @@ from CaO to SiO2.

TDB\_OXDEMO: @@ This means that for the IONIC\_LIQ phase the constituent Va should

TDB\_OXDEMO: @@ be suspended for systems with no degree of freedom with

TDB\_OXDEMO: @@ respect to oxygen

TDB\_OXDEMO: rej const

... the command in full is REJECT

PHASE: ion

SUBLATTICE NUMBER: 2

CONSTITUENT: va

VA IN IONIC\_LIQ:Y SUBLATTICE 2 REJECTED

CONSTITUENT:

TDB\_OXDEMO: l-sys

... the command in full is LIST\_SYSTEM

ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENTS/: CONSTITUENTS

GAS:G :CA CA101 CA2 O1SI1 O2 O2SI1 O2SI2 O3 SI SI2 SI3:

IONIC\_LIQ:Y :CA+2 SI+4:O-2 SIO4-4 SIO2:

> Ionic liquid mixture, modelled by the ionic two-sublattice model.

BCC A2 :CA SI:O VA:

CA2SIO4\_ALPHA :CA+2:SI+4:O-2:

> This is 2CaO.SiO2. Prototype Ca2[SiO4] (hP24, P63/mmc)

CA2SIO4\_ALPHA\_PRIME:I :CA+2:SI+4:O-2:

> This is 2CaO.SiO2. Prototype Sr2[SiO4] (oP52, Pnma)

CRISTOBALITE :SIO2:

> Prototype SiO2 (cF24, Fd3m)

DIAMOND\_FCC\_A4 :SI:O VA:

> Silicon (cF8, Fd-3m)

FCC A1 :CA SI:O VA:

HALITE:I :CA+2 VA:O-2:

> This is CaO and FeO (cI2, Im-3m)

HATRURITE :CA+2:SI+4:O-2:

> This is 3CaO.SiO2 (hR81, R3m)

HCP A3 :CA SI:VA:

LARNITE :CA+2:SI+4:O-2:

> This is 2CaO.SiO2 (metastable at 1 atm)

OLIVINE:I :CA+2:CA+2:SI+4:O-2:

> This is 2CaO.SiO2 and fayalite

PSEUDO\_WOLLASTONITE :CA+2:SI+4:O-2:

> This is CaO.SiO2 (mS120, C12/c1)

QUARTZ :SIO2:



```

> Prototype SiO2 (hP9, P3121 (rt) P6222 (ht))
RANKINITE :CA+2:SI+4:O-2:
> This is 3CaO.2SiO2 (mP48, P121/c1)
TRIDYMITE :SiO2:
> Prototype SiO2 (hP12, P63/mmc)
WOLLASTONITE:I :CA+2:SI+4:O-2:
> This is CaO.SiO2 (aP30, P-1)
TDB_OXDEMO:Hit RETURN to continue
TDB_OXDEMO: @@ The phase names may seem unfamiliar but this is due to the
TDB_OXDEMO: @@ attempt to create a general database. Thus lime (CaO) is
TDB_OXDEMO: @@ called HALITE which is the generic phase name for this structure.
TDB_OXDEMO: @@ HALITE is also the wudstite phase (FeO) and the periclase phase (MgO)
TDB_OXDEMO: @@ Note also that many phases are modelled with sublattices and
TDB_OXDEMO: @@ vacancies in order to allow for non-stoichiometry in higher
TDB_OXDEMO: @@ order system.
TDB_OXDEMO: @@ For simplicity we reject all phases except those we know
TDB_OXDEMO: @@ should be stable in this system.
TDB_OXDEMO: @@
TDB_OXDEMO: rej ph /all
... the command in full is REJECT
GAS:G IONIC_LIQ:Y BCC_A2
CA2SiO4_ALPHA CA2SiO4_ALPHA_PRIME:I CRISTOBALITE
DIAMOND_FCC_A4 FCC_A1 HALITE:I
HATRURITE HCP_A3 LARNITE
OLIVINE:I PSEUDO_WOLLASTONITE QUARTZ
RANKINITE TRIDYMITE WOLLASTONITE:I
REJECTED
TDB_OXDEMO: rest ph ionic_liq alpha_ca2sio4 alpha_prime cristobalite halite hatrurite
... the command in full is RESTORE
*** ALPHA_CA2SiO4 INPUT IGNORED
*** ALPHA_PRIME INPUT IGNORED
IONIC_LIQ:Y CRISTOBALITE HALITE:I
HATRURITE RESTORED
TDB_OXDEMO: rest ph larnite olivine pseudo_wollastonite quartz rankinite
... the command in full is RESTORE
LARNITE OLIVINE:I PSEUDO_WOLLASTONITE
QUARTZ RANKINITE RESTORED
TDB_OXDEMO: rest ph tridymite wollastonite
... the command in full is RESTORE
TRIDYMITE WOLLASTONITE:I RESTORED
TDB_OXDEMO: @@ To avoid complications we should also reject the Si+4 in the
TDB_OXDEMO: @@ first sublattice in the liquid phase. When there is oxygen present
TDB_OXDEMO: @@ all Si will form SiO2 or SiO4/-4. The Si+4 ion is needed only
TDB_OXDEMO: @@ for the liquid in systems without oxygen.
TDB_OXDEMO: rej const ionic_liq
... the command in full is REJECT
SUBLATTICE NUMBER: 1
CONSTITUENT: si+4
SI+4 IN IONIC_LIQ:Y SUBLATTICE 1 REJECTED
CONSTITUENT:
TDB_OXDEMO: l-sys
... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENTS/: CONSTITUENTS
IONIC_LIQ:Y :CA+2:O-2 SiO4-4 SiO2:
> Ionic liquid mixture, modelled by the ionic two-sublattice model.
CRISTOBALITE :SiO2:
> Prototype SiO2 (cF24, Fd3m)
HALITE:I :CA+2 VA:O-2:
> This is CaO and FeO (cI2, Im-3m)
HATRURITE :CA+2:SI+4:O-2:
> This is 3CaO.SiO2 (hR81, R3m)
LARNITE :CA+2:SI+4:O-2:
> This is 2CaO.SiO2 (metastable at 1 atm)
OLIVINE:I :CA+2:CA+2:SI+4:O-2:
> This is 2CaO.SiO2 and fayalite
PSEUDO_WOLLASTONITE :CA+2:SI+4:O-2:
> This is CaO.SiO2 (mS120, C12/c1)
QUARTZ :SiO2:
> Prototype SiO2 (hP9, P3121 (rt) P6222 (ht))
RANKINITE :CA+2:SI+4:O-2:
> This is 3CaO.2SiO2 (mP48, P121/c1)
TRIDYMITE :SiO2:
> Prototype SiO2 (hP12, P63/mmc)
WOLLASTONITE:I :CA+2:SI+4:O-2:
> This is CaO.SiO2 (aP30, P-1)
TDB_OXDEMO:Hit RETURN to continue
TDB_OXDEMO:
TDB_OXDEMO: get
... the command in full is GET_DATA
REINITIATING GES5 .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ...

List of references for assessed data

'A. Dinsdale, Private Communication, liquid and solid Al2O3,CaO, MgO'
'M. Hillert, B. Sundman and X. Wang, Calphad, 15 (1991), 53-58; CaO-SiO2'
'T.I. Barry, NPL, UK, Unpublished research 1987; liquid and solid SiO2'
'M. Hillert, B. Sundman and X. Wang, Metall Trans B, 21B (1990), 303-312;
CaO-SiO2'
'W. Huang, M. Hillert and X. Wang, Metall Mater Trans A, 26A (1995), 2293
-2231; CaO-MgO-SiO2'
-OK-
TDB_OXDEMO: @@ There is a miscibility gap in the ionic liquid close to SiO2.
TDB_OXDEMO: @@ In this database two composition sets will be created automatically
TDB_OXDEMO: @@ and one will have SiO2 as major constituent
TDB_OXDEMO:
TDB_OXDEMO: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3:
POLY_3: @@ Define more convenient components than the elements
POLY_3:
POLY_3: list-stat cps
... the command in full is LIST_STATUS
*** STATUS FOR ALL COMPONENTS
COMPONENT STATUS REF. STATE T(K) P(Pa)
VA ENTERED SER

```

```

CA          ENTERED  SER
O           ENTERED  SER
SI          ENTERED  SER
*** STATUS FOR ALL PHASES
PHASE      STATUS    DRIVING FORCE    MOLES
WOLLASTONITE  ENTERED    0.000000E+00    0.000000E+00
TRIDYMITITE  ENTERED    0.000000E+00    0.000000E+00
RANKINITE    ENTERED    0.000000E+00    0.000000E+00
QUARTZ       ENTERED    0.000000E+00    0.000000E+00
PSEUDO_WOLLASTONITE  ENTERED    0.000000E+00    0.000000E+00
OLIVINE      ENTERED    0.000000E+00    0.000000E+00
LARNITE      ENTERED    0.000000E+00    0.000000E+00
HATRURITE    ENTERED    0.000000E+00    0.000000E+00
HALITE       ENTERED    0.000000E+00    0.000000E+00
CRISTOBALITE ENTERED    0.000000E+00    0.000000E+00
IONIC_LIQ#2  ENTERED    0.000000E+00    0.000000E+00
IONIC_LIQ    ENTERED    0.000000E+00    0.000000E+00
*** STATUS FOR ALL SPECIES
CA          ENTERED  0      ENTERED  O2SI2  ENTERED  SI3      ENTERED
CA+2        ENTERED  0-2    ENTERED  O3      ENTERED  SIO2     ENTERED
CA101       ENTERED  O1S11  ENTERED  SI       ENTERED  SIO4-4   ENTERED
CA2          ENTERED  O2      ENTERED  SI+4     ENTERED  VA        ENTERED
CAO          ENTERED  O2-2    ENTERED  SI2      ENTERED  VA-2     ENTERED
E-          ENTERED  O2SI1   ENTERED  SI2O7-6  ENTERED
POLY_3: def-com cao sio2 o
... the command in full is DEFINE_COMPONENTS
POLY_3: l-st cps
... the command in full is LIST_STATUS
*** STATUS FOR ALL COMPONENTS
COMPONENT   STATUS    REF. STATE    T(K)          P(Pa)
VA           ENTERED  SER
CAO          ENTERED  SER
SIO2         ENTERED  SER
O            ENTERED  SER
*** STATUS FOR ALL PHASES
PHASE      STATUS    DRIVING FORCE    MOLES
WOLLASTONITE  ENTERED    0.000000E+00    0.000000E+00
TRIDYMITITE  ENTERED    0.000000E+00    0.000000E+00
RANKINITE    ENTERED    0.000000E+00    0.000000E+00
QUARTZ       ENTERED    0.000000E+00    0.000000E+00
PSEUDO_WOLLASTONITE  ENTERED    0.000000E+00    0.000000E+00
OLIVINE      ENTERED    0.000000E+00    0.000000E+00
LARNITE      ENTERED    0.000000E+00    0.000000E+00
HATRURITE    ENTERED    0.000000E+00    0.000000E+00
HALITE       ENTERED    0.000000E+00    0.000000E+00
CRISTOBALITE ENTERED    0.000000E+00    0.000000E+00
IONIC_LIQ#2  ENTERED    0.000000E+00    0.000000E+00
IONIC_LIQ    ENTERED    0.000000E+00    0.000000E+00
*** STATUS FOR ALL SPECIES
CA          ENTERED  0      ENTERED  O2SI2  ENTERED  SI3      ENTERED
CA+2        ENTERED  0-2    ENTERED  O3      ENTERED  SIO2     ENTERED
CA101       ENTERED  O1S11  ENTERED  SI       ENTERED  SIO4-4   ENTERED
CA2          ENTERED  O2      ENTERED  SI+4     ENTERED  VA        ENTERED
CAO          ENTERED  O2-2    ENTERED  SI2      ENTERED  VA-2     ENTERED
E-          ENTERED  O2SI1   ENTERED  SI2O7-6  ENTERED
POLY_3:Hit RETURN to continue
POLY_3: s-c t=2000,p=1e5,n=1,w(sio2)=.9
... the command in full is SET_CONDITION
POLY_3: l-c
... the command in full is LIST_CONDITIONS
T=2000, P=1E5, N=1, W(SIO2)=0.9
DEGREES OF FREEDOM 1
POLY_3: @@ There is one degree of freedom due to the oxygen. As the oxygen content
POLY_3: @@ is determined by the Ca/Si ration there is no possibility to vary
POLY_3: @@ the oxygen content in this system independently. Thus the
POLY_3: @@ oxygen potential can be set to any value (larger than zero).
POLY_3: s-c ac(o)=1
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated      2023 grid points in      0 s
51 ITS, CPU TIME USED 0 SECONDS
POLY_3:
POLY_3: @@ Option N is used to include information on the
POLY_3: @@ constitution of the phases.
POLY_3: l-e screen
... the command in full is LIST_EQUILIBRIUM
Options /VWCS/: n
Output from POLY-3, equilibrium = 1, label A0 , database: OXDEMO

Conditions:
T=2000, P=1E5, N=1, W(SIO2)=0.9, AC(O)=1
DEGREES OF FREEDOM 0

Temperature 2000.00 K ( 1726.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 5.96571E+01
Total Gibbs energy -1.10541E+06, Enthalpy -7.53274E+05, Volume 0.00000E+00

Component      Moles      W-Fraction Activity Potential Ref.stat
CAO             1.0638E-01  1.0000E-01  6.4224E-25 -9.2632E+05 SER
SIO2            8.9362E-01  9.0000E-01  3.7467E-30 -1.1267E+06 SER
O               0.0000E+00  3.6248E-18  1.0000E+00  0.0000E+00 SER

IONIC_LIQ#2      Status ENTERED Driving force 0.0000E+00
Moles 6.7245E-01, Mass 4.0314E+01, Volume fraction 0.0000E+00 Mass fractions:
SIO2 9.69163E-01 CAO 3.08366E-02 O 0.00000E+00
Constitution:
Sublattice 1, Number of sites 6.8156E-02
CA+2 1.00000E+00
Sublattice 2, Number of sites 2.0000E+00
SIO2 9.82793E-01 SIO4-4 1.68709E-02 O-2 3.36172E-04

IONIC_LIQ      Status ENTERED Driving force 0.0000E+00
Moles 3.2755E-01, Mass 1.9343E+01, Volume fraction 0.0000E+00 Mass fractions:
SIO2 7.55851E-01 CAO 2.44149E-01 O 0.00000E+00
Constitution:
Sublattice 1, Number of sites 6.9176E-01
CA+2 1.00000E+00
Sublattice 2, Number of sites 2.0000E+00
SIO2 8.26780E-01 SIO4-4 1.72662E-01 O-2 5.57209E-04
POLY_3:Hit RETURN to continue
POLY_3: @@ The result shows the expected miscibility gap. However, in some
POLY_3: @@ cases the first calculation may fail. In such cases try to simplify the

```

```

POLY_3: @@ calculation by suspending all phases but the important ones.
POLY_3: @@ Save the results so far on file
POLY_3:
POLY_3: save tcex17 y
... the command in full is SAVE_WORKSPACES
POLY_3: @@ Set the axis
POLY_3: s-a-v 1 w(sio2)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: 1
Increment /.025/: .025
POLY_3: s-a-v 2 t
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 1500
Max value /1/: 3500
Increment /50/: 20
POLY_3: save tcex17 Y
... the command in full is SAVE_WORKSPACES
POLY_3: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16

Phase region boundary 1 at: 9.053E-01 1.959E+03
IONIC_LIQ
IONIC_LIQ#2
** CRISTOBALITE
Calculated 19 equilibria

Phase region boundary 2 at: 9.053E-01 1.959E+03
IONIC_LIQ
IONIC_LIQ#2
** CRISTOBALITE
Calculated 16 equilibria

Phase region boundary 3 at: 9.053E-01 1.959E+03
IONIC_LIQ
IONIC_LIQ#2
** CRISTOBALITE
Calculated 19 equilibria

Phase region boundary 4 at: 9.053E-01 1.959E+03
IONIC_LIQ
IONIC_LIQ#2
** CRISTOBALITE
Calculated 16 equilibria

Phase region boundary 5 at: 9.053E-01 1.959E+03
IONIC_LIQ
IONIC_LIQ#2
** CRISTOBALITE
Calculated 19 equilibria

Phase region boundary 6 at: 9.053E-01 1.959E+03
IONIC_LIQ
IONIC_LIQ#2
** CRISTOBALITE
Calculated 16 equilibria

Phase region boundary 7 at: 9.053E-01 1.959E+03
IONIC_LIQ
IONIC_LIQ#2
** CRISTOBALITE
Calculated 19 equilibria

Phase region boundary 8 at: 9.053E-01 1.959E+03
IONIC_LIQ
IONIC_LIQ#2
** CRISTOBALITE
Calculated 16 equilibria

Phase region boundary 9 at: 8.835E-01 2.137E+03
** IONIC_LIQ
IONIC_LIQ#2
Calculated. 10 equilibria

Phase region boundary 10 at: 8.348E-01 1.959E+03
** IONIC_LIQ
IONIC_LIQ#2
** CRISTOBALITE

Phase region boundary 11 at: 9.882E-01 1.959E+03

```

IONIC\_LIQ#2  
 \*\* CRISTOBALITE  
 Calculated 18 equilibria  
 Phase region boundary 12 at: 8.695E-01 1.959E+03  
 IONIC\_LIQ  
 \*\* CRISTOBALITE  
 Calculated. 12 equilibria  
 Phase region boundary 13 at: 8.222E-01 1.744E+03  
 IONIC\_LIQ  
 \*\* CRISTOBALITE  
 \*\* TRIDYMITE  
 Phase region boundary 14 at: 8.222E-01 1.744E+03  
 IONIC\_LIQ  
 \*\* TRIDYMITE  
 Calculated. 3 equilibria  
 Phase region boundary 15 at: 8.175E-01 1.714E+03  
 IONIC\_LIQ  
 \*\* PSEUDO\_WOLLASTONITE  
 \*\* TRIDYMITE  
 Phase region boundary 16 at: 5.740E-01 1.714E+03  
 IONIC\_LIQ  
 \*\* PSEUDO\_WOLLASTONITE  
 Calculated. 22 equilibria  
 Phase region boundary 17 at: 4.813E-01 1.727E+03  
 IONIC\_LIQ  
 \*\* PSEUDO\_WOLLASTONITE  
 \*\* RANKINITE  
 Phase region boundary 18 at: 4.309E-01 1.727E+03  
 IONIC\_LIQ  
 \*\* RANKINITE  
 Calculated. 3 equilibria  
 Phase region boundary 19 at: 4.184E-01 1.749E+03  
 IONIC\_LIQ  
 \*\* LARNITE  
 \*\* RANKINITE  
 Phase region boundary 20 at: 3.845E-01 1.749E+03  
 IONIC\_LIQ  
 \*\* LARNITE  
 Calculated. 39 equilibria  
 Phase region boundary 21 at: 3.459E-01 2.160E+03  
 IONIC\_LIQ  
 \*\* HATRURITE  
 \*\* LARNITE  
 Phase region boundary 22 at: 3.032E-01 2.160E+03  
 IONIC\_LIQ  
 \*\* HATRURITE  
 Calculated. 16 equilibria  
 Phase region boundary 23 at: 2.736E-01 2.422E+03  
 IONIC\_LIQ  
 \*\* HALITE  
 \*\* HATRURITE  
 Phase region boundary 24 at: 1.433E-01 2.422E+03  
 IONIC\_LIQ  
 \*\* HALITE  
 Calculated 53 equilibria  
 Phase region boundary 25 at: 1.327E-01 2.422E+03  
 \*\* HALITE  
 HATRURITE  
 Calculated.. 48 equilibria  
 Terminating at axis limit.  
 Phase region boundary 26 at: 3.061E-01 2.160E+03  
 \*\* HATRURITE  
 LARNITE  
 Calculated.. 34 equilibria  
 Terminating at axis limit.  
 Phase region boundary 27 at: 3.828E-01 1.749E+03  
 \*\* LARNITE  
 RANKINITE  
 Calculated.. 14 equilibria  
 Terminating at axis limit.  
 Phase region boundary 28 at: 4.671E-01 1.727E+03  
 PSEUDO\_WOLLASTONITE  
 \*\* RANKINITE  
 Calculated.. 13 equilibria  
 Terminating at axis limit.  
 Phase region boundary 29 at: 7.627E-01 1.714E+03  
 \*\* PSEUDO\_WOLLASTONITE  
 TRIDYMITE  
 Calculated.. 12 equilibria  
 Terminating at axis limit.  
 Phase region boundary 30 at: 1.000E+00 1.744E+03  
 CRISTOBALITE  
 \*\* TRIDYMITE  
 Phase region boundary 31 at: 8.574E-01 1.959E+03  
 \*\* IONIC\_LIQ  
 IONIC\_LIQ#2  
 Calculated. 35 equilibria  
 Terminating at known equilibrium  
 Phase region boundary 32 at: 8.835E-01 2.137E+03  
 \*\* IONIC\_LIQ  
 IONIC\_LIQ#2  
 Calculated 6 equilibria  
 Phase region boundary 33 at: 8.835E-01 2.137E+03  
 \*\* IONIC\_LIQ

```

      IONIC_LIQ#2
Calculated.                10 equilibria
Terminating at known equilibrium

Phase region boundary 34 at: 8.835E-01 2.137E+03
** IONIC_LIQ
      IONIC_LIQ#2
Calculated.                7 equilibria

Phase region boundary 35 at: 8.835E-01 2.137E+03
** IONIC_LIQ
      IONIC_LIQ#2
Calculated.                10 equilibria
Terminating at known equilibrium

Phase region boundary 36 at: 8.835E-01 2.137E+03
** IONIC_LIQ
      IONIC_LIQ#2
Calculated.                25 equilibria
Terminating at known equilibrium

Phase region boundary 37 at: 8.835E-01 2.137E+03
** IONIC_LIQ
      IONIC_LIQ#2
Calculated.                10 equilibria
Terminating at known equilibrium

Phase region boundary 38 at: 8.835E-01 2.137E+03
** IONIC_LIQ
      IONIC_LIQ#2
Calculated.                6 equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex17\tcex
17.POLY3
CPU time for mapping                2 seconds

```

POLY\_3:

POLY\_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-d-a x w-p sio2

... the command in full is SET\_DIAGRAM\_AXIS

POST: s-d-a y t-c

... the command in full is SET\_DIAGRAM\_AXIS

POST:

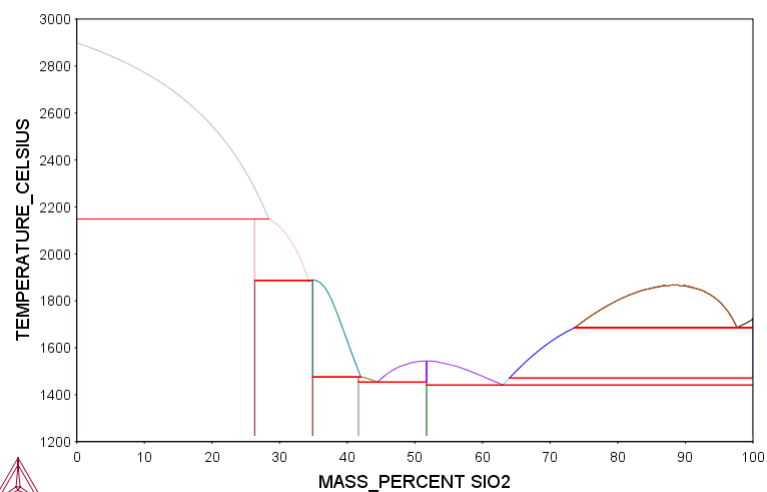
POST: set-title example 17a

POST: plot

... the command in full is PLOT DIAGRAM

example 17a

2016.05.16.13.35.56  
OXDEMO: CAO, SIO2, O  
P=1E5, N=1, AC(O)=1



POST:

POST:Hit RETURN to continue

POST: @@ Identify the phases with labels

POST: s-lab

... the command in full is SET\_LABEL\_CURVE\_OPTION

CURVE LABEL OPTION (A, B, C, D, E, F OR N) /N/: f

POST:

POST: set-title example 17b

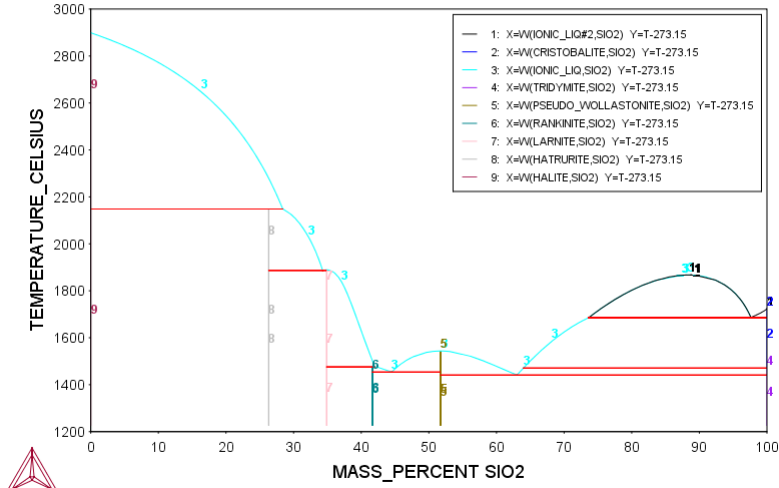
POST:

POST: plot

... the command in full is PLOT\_DIAGRAM

example 17b

2016.05.16 13:35:57  
OXDEMO: CAO, SiO2, O  
P=1E5, N=1, AC(O)=1



POST:  
POST: set-inter  
... the command in full is SET\_INTERACTIVE\_MODE  
POST:

## tcex18

About Software (build 9533) running on WinNT 64-bit wordlength  
Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118  
License library version: 8.5.1.0017  
Linked: Mon May 16 09:31:44 2016

SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex18\tcex18.TCM" set-echo

SYS: @@  
SYS: @@ Calculation  
SYS: @@ of the A3 temperature  
SYS: @@ of a steel and the influence  
SYS: @@ of each alloying element on  
SYS: @@ this temperature  
SYS: @@  
SYS: @@  
SYS: @@ A3 temperature is the temperature where ferrite starts to form from  
SYS: @@ austenite. One can easily read A3 from Fe-C phase diagram. But for  
SYS: @@ complex multicomponent steels, no simple diagram can be used.  
SYS: @@ This example shows how to calculate the A3 temperature of a steel.  
SYS: @@ Using the facility in POLY, it is easy to find out the influence  
SYS: @@ of each alloying element on A3 temperature. This information is  
SYS: @@ useful if one wants to modify the compositions of a steel but keep  
SYS: @@ A3 unchanged.  
SYS: @@  
SYS: set-log ex18,,  
SYS: go p-3  
... the command in full is GOTO\_MODULE

POLY version 3.32  
POLY\_3: def-mat  
... the command in full is DEFINE\_MATERIAL  
THERMODYNAMIC DATABASE module  
Current database: Steels/Fe-Alloys v8.0

VA DEFINED  
L12\_FCC B2\_BCC B2\_VACANCY  
HIGH\_SIGMA DICTRA\_FCC\_A1 REJECTED

Database /TCFE8/: tcfe7  
Current database: Steels/Fe-Alloys v7.0

VA DEFINED  
L12\_FCC B2\_BCC B2\_VACANCY  
HIGH\_SIGMA DICTRA\_FCC\_A1 REJECTED

Major element or alloy: fe  
Composition input in mass (weight) percent? /Y/:  
1st alloying element: cr 1.5 mn .5 c .3 si .3 nb .1  
Next alloying element:  
Temperature (C) /1000/: 1100

VA DEFINED  
L12\_FCC B2\_BCC B2\_VACANCY  
HIGH\_SIGMA DICTRA\_FCC\_A1 REJECTED  
REINITIATING GES5 .....  
... the command in full is DEFINE\_ELEMENTS  
FE DEFINED  
... the command in full is DEFINE\_ELEMENTS  
CR DEFINED  
... the command in full is DEFINE\_ELEMENTS  
MN DEFINED  
... the command in full is DEFINE\_ELEMENTS  
C DEFINED  
... the command in full is DEFINE\_ELEMENTS  
SI DEFINED  
... the command in full is DEFINE\_ELEMENTS  
NB DEFINED

This database has following phases for the defined system

GAS:G	LIQUID:L	BCC_A2
FCC_A1	HCP_A3	DIAMOND_FCC_A4
GRAPHITE	CEMENTITE	M23C6
M7C3	M6C	M5C2
M3C2	KSI_CARBIDE	A1_KAPPA
KAPPA	Z_PHASE	FE4N_LP1
FECN_CHI	SIGMA	MU_PHASE
CHI_A12	LAVES_PHASE_C14	M3SI
G_PHASE	CR3SI	FE2SI
MSI	M5SI3	NBNi3
AL4C3	FE8SI2C	SIC

Reject phase(s) /NONE/: ?

Reject phase(s)

This is a question generated by the database allowing the user to select the phases. Normally, all phases should be included and the user just presses <RETURN>.

If a phase is to be rejected, the name of the phase must be supplied. Several phase names can be specified in one line.

It is possible to reject all phase by giving an asterisk "\*". If the number of phases to be included is much smaller than the total number of phases, it may be convenient to first reject all phases and then restore just those that should be included.

Note: This question will be repeated until the user press <RETURN> after rejected all undesired phases or an asterisk "\*".

Reject phase(s) /NONE/: \*

GAS:G	LIQUID:L	BCC_A2
FCC_A1	HCP_A3	DIAMOND_FCC_A4
GRAPHITE	CEMENTITE	M23C6
M7C3	M6C	M5C2
M3C2	KSI_CARBIDE	A1_KAPPA
KAPPA	Z_PHASE	FE4N_LP1
FECN_CHI	SIGMA	MU_PHASE
CHI_A12	LAVES_PHASE_C14	M3SI
G_PHASE	CR3SI	FE2SI
MSI	M5SI3	NBNi3

```

AL4C3          FE8SI2C          SIC
REJECTED
Restore phase(s):: liq fcc_a1 bcc_a2 hcp_a3 graphite cementite m23 m7
LIQUID:L        FCC_A1          BCC_A2
HCP_A3          GRAPHITE        CEMENTITE
M23C6           M7C3   RESTORED
Restore phase(s): /NONE/

.....

The following phases are retained in this system:

LIQUID:L        BCC_A2          FCC_A1
HCP_A3          GRAPHITE        CEMENTITE
M23C6           M7C3

.....

OK? /Y/: Y
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

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-OK-
Should any phase have a miscibility gap check? /N/: N
Using global minimization procedure
Calculated          10008 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution          0 s, total time          0 s
POLY_3:
POLY_3:
POLY_3:
POLY_3: @@ In the TCFE database the number of phases is very large.
POLY_3: @@ It is strongly recommended that one rejects all phases
POLY_3: @@ that one knows should not be stable
POLY_3:
POLY_3: 1-e,,,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium =          1, label A0 , database: TCFE7

Conditions:
T=1373.15, W(CR)=1.5E-2, W(MN)=5E-3, W(C)=3E-3, W(SI)=3E-3, W(NB)=1E-3,
P=1E5, N=1
DEGREES OF FREEDOM 0

```



Temperature 1373.15 K ( 1100.00 C), Pressure 1.000000E+05  
Number of moles of components 1.00000E+00, Mass in grams 5.50375E+01  
Total Gibbs energy -7.21999E+04, Enthalpy 4.05686E+04, Volume 7.32058E-06

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
C	1.3747E-02	3.0000E-03	1.0740E-02	-5.1763E+04	SER
CR	1.5877E-02	1.5000E-02	1.3123E-04	-1.0205E+05	SER
FE	9.5890E-01	9.7300E-01	2.0390E-03	-7.0732E+04	SER
MN	5.0091E-03	5.0000E-03	4.2846E-06	-1.4112E+05	SER
NB	5.9240E-04	1.0000E-03	1.3310E-07	-1.8076E+05	SER
SI	5.8788E-03	3.0000E-03	1.1131E-08	-2.0909E+05	SER

FCC A1 Status ENTERED Driving force 0.0000E+00  
Moles 9.9900E-01, Mass 5.4984E+01, Volume fraction 9.9904E-01 Mass fractions:  
FE 9.73932E-01 MN 5.00479E-03 C 2.89608E-03  
CR 1.50122E-02 SI 3.00290E-03 NB 1.51584E-04

FCC A1#2 Status ENTERED Driving force 0.0000E+00  
Moles 1.0011E-03, Mass 5.3091E-02, Volume fraction 9.5720E-04 Mass fractions:  
NB 8.79676E-01 FE 7.33072E-03 MN 3.71964E-05  
C 1.10624E-01 CR 2.33143E-03 SI 1.24275E-09

POLY\_3:Hit RETURN to continue

POLY\_3: @@ Two FCC phases are stable, one with mainly Fe and

POLY\_3: @@ one with mainly Nb and C, which is the NbC carbide.

POLY\_3: @@ The second fcc is called FCC#2. The digit after # is

POLY\_3: @@ called composition set but can be ignored if it is unity.

POLY\_3:

POLY\_3: li-st

... the command in full is LIST\_STATUS

Option /CPS/: CPS

\*\*\* STATUS FOR ALL COMPONENTS

COMPONENT	STATUS	REF. STATE	T(K)	P(Pa)
VA	ENTERED	SER		
C	ENTERED	SER		
CR	ENTERED	SER		
FE	ENTERED	SER		
MN	ENTERED	SER		
NB	ENTERED	SER		
SI	ENTERED	SER		

\*\*\* STATUS FOR ALL PHASES

PHASE	STATUS	DRIVING FORCE	MOLES
FCC A1#2	ENTERED	0.000000E+00	1.001053E-03
FCC_A1	ENTERED	0.000000E+00	9.989989E-01
BCC_A2	ENTERED	-1.877374E-02	0.000000E+00
LIQUID	ENTERED	-2.093926E-01	0.000000E+00
HCP_A3	ENTERED	-3.238293E-01	0.000000E+00
HCP A3#2	ENTERED	-3.238293E-01	0.000000E+00
M23C6	ENTERED	-3.975771E-01	0.000000E+00
CEMENTITE	ENTERED	-4.579912E-01	0.000000E+00
M7C3	ENTERED	-6.050859E-01	0.000000E+00
GRAPHITE	ENTERED	-2.504689E+00	0.000000E+00

\*\*\* STATUS FOR ALL SPECIES

C	ENTERED	C4	ENTERED	CR	ENTERED	NB	ENTERED
C2	ENTERED	C5	ENTERED	FE	ENTERED	SI	ENTERED
C3	ENTERED	C60	ENTERED	MN	ENTERED	VA	ENTERED

POLY\_3:

POLY\_3: @@ Fcc appears twice on the list above. The HCP phase also has

POLY\_3: @@ two composition sets.

POLY\_3:

POLY\_3: @@ This result looks reasonable, save it on a file

POLY\_3: save tcex18 y

... the command in full is SAVE\_WORKSPACES

POLY\_3:

POLY\_3: @@ Now calculate when bcc (ferrite) begins to form

POLY\_3: @@ using the COMPUTE-TRANSITION command

POLY\_3: c-t

... the command in full is COMPUTE TRANSITION

This command is a combination of CHANGE STATUS and SET\_CONDITION

to calculate directly when a phase may form by releasing one condition.

Phase to form: bcc\_a2

You must release one of these conditions

T=1373.15, W(CR)=1.5E-2, W(MN)=5E-3, W(C)=3E-3, W(SI)=3E-3, W(NB)=1E-3,  
P=1E5, N=1 DEGREES OF FREEDOM 0

Give the state variable to be removed /T/: t

Testing POLY result by global minimization procedure

Calculated 10008 grid points in 1 s

To form BCC\_A2 the condition is set to T=1071.60881565

POLY\_3:Hit RETURN to continue

POLY\_3: @@ We may expect BCC to form at a lower temperature, because sometimes

POLY\_3: @@ a higher temperature is found as there is a delta-ferrite stable

POLY\_3: @@ at high temperatures.

POLY\_3: @@

POLY\_3: @@ Calculate again the equilibrium at lower temperature. You can

POLY\_3: @@ do this by just a SET-COND T=... command but then the temperature must

POLY\_3: @@ be given in Kelvin. You can use the DEF-MAT command to do this

POLY\_3: @@ in Celsius

POLY\_3: def-mat

... the command in full is DEFINE\_MATERIAL

Same elements as before? /Y/: Y

Mass (weight) percent of C /.3/: .3

Mass (weight) percent of CR /1.5/: 1.5

Mass (weight) percent of MN /.5/: .5

Mass (weight) percent of NB /.1/: .1

Mass (weight) percent of SI /.3/: .3

Temperature (C) /798/: 800

Using global minimization procedure

Calculated 10008 grid points in 0 s

Found the set of lowest grid points in 0 s

Calculated POLY solution 0 s, total time 0 s

POLY\_3: l-e,,,

... the command in full is LIST\_EQUILIBRIUM

Output from POLY-3, equilibrium = 1, label A0 , database: TCFE7

Conditions:

T=1073.15, W(CR)=1.5E-2, W(MN)=5E-3, W(C)=3E-3, W(SI)=3E-3, W(NB)=1E-3,

P=1E5, N=1

DEGREES OF FREEDOM 0

Temperature 1073.15 K ( 800.00 C), Pressure 1.000000E+05

Number of moles of components 1.00000E+00, Mass in grams 5.50375E+01

Total Gibbs energy -4.87895E+04, Enthalpy 3.03117E+04, Volume 7.17692E-06

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
-----------	-------	------------	----------	-----------	----------

```

C          1.3747E-02   3.0000E-03   4.4068E-02  -2.7857E+04  SER
CR         1.5877E-02   1.5000E-02   3.5554E-04  -7.0863E+04  SER
FE         9.5890E-01   9.7300E-01   4.8677E-03  -4.7515E+04  SER
MN         5.0091E-03   5.0000E-03   8.2064E-06  -1.0449E+05  SER
NB         5.9240E-04   1.0000E-03   2.9934E-09  -1.7512E+05  SER
SI         5.8788E-03   3.0000E-03   8.9756E-10  -1.8587E+05  SER

FCC A1          Status ENTERED      Driving force  0.0000E+00
Moles 9.9870E-01, Mass 5.4971E+01, Volume fraction 9.9878E-01  Mass fractions:
FE  9.74156E-01  MN  5.00593E-03  C   2.86369E-03
CR  1.49685E-02  SI  3.00361E-03  NB  2.74704E-06

FCC A1#2          Status ENTERED      Driving force  0.0000E+00
Moles 1.2984E-03, Mass 6.6134E-02, Volume fraction 1.2211E-03  Mass fractions:
NB  8.29930E-01  CR  4.11711E-02  MN  7.37925E-05
C   1.16301E-01  FE  1.25236E-02  SI  1.74994E-10

POLY_3:
POLY_3: @@ Try a slightly different COMPUTE-TRANSITION command.
POLY_3: @@ This finds the first phase change in the specified direction.
POLY_3: c-t
... the command in full is COMPUTE_TRANSITION
This command is a combination of CHANGE_STATUS and SET_CONDITION
to calculate directly when a phase may form by releasing one condition.
Phase to form: any
You must release one of these conditions
T=1073.15, W(CR)=1.5E-2, W(MN)=5E-3, W(C)=3E-3, W(SI)=3E-3, W(NB)=1E-3,
P=1E5, N=1  DEGREES OF FREEDOM 0
Give the state variable to be removed /T/: t
Estimated change (with sign) /1/: ?

Estimated change (with sign)

A given varying direction sign and an estimated change of the released
condition, in this case X(FE), must be given here: a negative sign means
at a lower value of the released condition any new phase is to be found,
and a positive sign at a higher value; an estimated change of the released
condition implies where any new phase is expected (but it is only estimated
value, so any value within its reasonable scale would be enough).

For instance, if a combination of -.02 is input, the following message may
come up (after a successful calculation):
    To form BCC_A2#1 the condition is set to X(FE)=.493708756187

This calculated value will then be assign as the parameter of that removed
condition, in this case, the X(FE) variable. So the following message will
be shown on the screen, if the LIST_CONDITIONS command is typed:
    P=100000, T=800, N=1, X(FE)=4.93708756E-1
    DEGREES OF FREEDOM 0

Estimated change (with sign) /1/: -1
Testing POLY result by global minimization procedure
Calculated      10008 grid points in      0 s
To form BCC_A2#1 the condition is set to T=1071.60881565
POLY_3: show t
... the command in full is SHOW_VALUE
T=1071.6088
POLY_3: @@ The transition temperature to form BCC is the same.
POLY_3: @@ If we want it in Celsius enter a function for that.
POLY_3: enter fun tc=t-273;
... the command in full is ENTER_SYMBOL
POLY_3: show tc
... the command in full is SHOW_VALUE
TC=798.60882
POLY_3:
POLY_3:Hit RETURN to continue
POLY_3: @@ This is the minimum temperature for hardening because below this
POLY_3: @@ temperature ferrite will form from austenite. Check how a small
POLY_3: @@ change of the composition can change this temperature. We must
POLY_3: @@ then set bcc as fix and release the condition on the temperature.
POLY_3: c-st p bcc_a2=fix 0
... the command in full is CHANGE_STATUS
POLY_3: s-c t=none
... the command in full is SET_CONDITION
POLY_3: @@ The change of the calculated temperature for a small change of
POLY_3: @@ the amount of a component can be calculated as a derivative
POLY_3: @@ using the dot "." between the calculated variable and the condition.
POLY_3: sh t.w(mn)
... the command in full is SHOW_VALUE
T.W(MN)=-2592.1917
POLY_3: sh t.w(cr)
... the command in full is SHOW_VALUE
T.W(CR)=-781.45507
POLY_3: sh t.w(nb)
... the command in full is SHOW_VALUE
T.W(NB)=3005.9537
POLY_3: sh t.w(c)
... the command in full is SHOW_VALUE
T.W(C)=-21796.295
POLY_3: sh t.w(si)
... the command in full is SHOW_VALUE
T.W(SI)=2990.1116
POLY_3:Hit RETURN to continue
POLY_3: @@ A negative value means the temperature will decrease if the
POLY_3: @@ amount is increased. Check for Mn
POLY_3: s-c w(mn)
... the command in full is SET_CONDITION
Value /.005/:.01
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated      10008 grid points in      0 s
9 ITS, CPU TIME USED  0 SECONDS
POLY_3: sh t
... the command in full is SHOW_VALUE
T=1058.9661
POLY_3:Hit RETURN to continue
POLY_3: @@ The temperature decreased from 1072 to 1059 i.e. 13 degrees.
POLY_3: @@ According to the derivatives calculated above, one could increase
POLY_3: @@ the temperature with the same amount by increasing the amount of Si
POLY_3: @@ 2592/2990=0.8669 times of the change in Mn i.e. from 0.3 to 0.733 %
POLY_3: s-c w(si)
... the command in full is SET_CONDITION

```

```
Value /.003/: .00733
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated      10008 grid points in      0 s
      10 ITS, CPU TIME USED   0 SECONDS
POLY_3: sh t
... the command in full is SHOW_VALUE
T=1070.73
POLY_3: @@ The facility to calculate these derivatives is a powerful feature
POLY_3: @@ in order to find the best way to obtain a certain property of a material.
POLY_3: set-inter
... the command in full is SET_INTERACTIVE
POLY_3:
```

tcex19A

```
AboutMACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19A\tcex19A.TCM"SYS: set-echo
SYS: @@
SYS: @@
SYS: @@ Mapping of univariant equilibria with the liquid in Al-Cu-Si
SYS: @@ Part A: step-by-step calculation
SYS: @@
SYS: set-log ex19a,,
SYS: go da
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
L12_FCC B2_BCC B2_VACANCY
HIGH_SIGMA DICTRA_FCC_A1 REJECTED
TDB_TCFE8: sw USER tcex19_cost2
... the command in full is SWITCH_DATABASE
Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

VA /- DEFINED
TDB_USER: d-sys
... the command in full is DEFINE_SYSTEM
ELEMENTS: cu al si
CU AL SI
DEFINED
TDB_USER: l-s c
... the command in full is LIST_SYSTEM
LIQUID:L :AL CU SI:
ALCE_AMORPHOUS :AL:
ALCUZN_T :AL:CU VA:
ALCU_DELTA :AL:CU:
ALCU_EPSILON :AL CU:CU:
ALCU_ETA :AL CU:CU:
ALCU_PRIME :AL:CU:
ALCU_THETA :AL:AL CU:
ALCU_ZETA :AL:CU:
ALLI :AL:VA:
ALMO :AL:AL:
ALM_D019 :AL:AL:
ALND_AMORPHOUS :AL:
ALTI :AL:AL:
BCC_A2 :AL CU SI:VA:
BCC_B2 :AL CU SI:AL CU SI:VA:
BCT_A5 :AL:
CBCC_A12 :AL SI:VA:
CR3SI_A15 :SI:AL SI:
CRSI2 :SI:SI:
CU19SI6_ETA :CU:SI:
CU33SI7_DELTA :CU:SI:
CU4SI_EPSILON :CU:SI:
CU56SI11_GAMMA :CU:SI:
CU6Y :CU:CU2:
CUB_A13 :AL SI:VA:
CUB_A15 :SI:AL SI:
DIAMOND_A4 :AL SI:
FCC_A1 :AL CU SI:VA:
GAMMA_D83 :AL:AL CU:CU:
GAMMA_H :AL:AL CU:CU:
HCP_A3 :AL CU SI:VA:
HCP_ZN :AL CU SI:VA:
LAVES_C14 :AL CU:AL CU:
LAVES_C15 :AL CU SI:AL CU SI:
LAVES_C36 :AL CU:AL CU:
SIV3 :SI:SI:
TDB_USER: get
... the command in full is GET_DATA
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
Reference REF1 missing close to line 641
Reference REF1 missing close to line 643
Reference REF1 missing close to line 645
FUNCTIONS ....

List of references for assessed data

'COST2 - TCOST507 Light Alloys Database (Version 2.1), provided by TCSAB,
1999/2003. '
-OK-
TDB_USER: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3: s-c t=1300,p=101325,n=1
... the command in full is SET_CONDITION
POLY_3: l-c
... the command in full is LIST_CONDITIONS
T=1300, P=1.01325E5, N=1
DEGREES OF FREEDOM 2
POLY_3: s-c x(si)=.25,x(al)=.2
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 16220 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY_3: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: vwcs
Output from POLY-3, equilibrium = 1, label A0 , database: USER

Conditions:
```

T=1300, P=1.01325E5, N=1, X(SI)=0.25, X(AL)=0.2  
DEGREES OF FREEDOM 0

Temperature 1300.00 K ( 1026.85 C), Pressure 1.013250E+05  
Number of moles of components 1.00000E+00, Mass in grams 4.73679E+01  
Total Gibbs energy -8.02595E+04, Enthalpy 3.22931E+04, Volume 0.00000E+00

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
AL	2.0000E-01	1.1393E-01	5.1836E-05	-1.0666E+05	SER
CU	5.5000E-01	7.3785E-01	4.1349E-04	-8.4211E+04	SER
SI	2.5000E-01	1.4823E-01	9.3957E-03	-5.0450E+04	SER

LIQUID Status ENTERED Driving force 0.0000E+00  
Moles 1.0000E+00, Mass 4.7368E+01, Volume fraction 0.0000E+00 Mass fractions:  
CU 7.37847E-01 SI 1.48228E-01 AL 1.13925E-01

POLY\_3: Hit RETURN to continue

POLY\_3: @@ we want to calculate the monovariant lines with liquid. Select

POLY\_3: @@ two compositions and the temperature as axis

POLY\_3: s-a-v 1 x(al)

... the command in full is SET\_AXIS\_VARIABLE

Min value /0/: 0

Max value /1/: 1

Increment /.025/: .01

POLY\_3: s-a-v 2 x(si)

... the command in full is SET\_AXIS\_VARIABLE

Min value /0/: 0

Max value /1/: 1

Increment /.025/: .01

POLY\_3: s-a-v 3 t 500 2000 25

... the command in full is SET\_AXIS\_VARIABLE

POLY\_3: @@Set liquid as "present", otherwise all monovariant lines will be calculated.

POLY\_3: adva

... the command in full is ADVANCED\_OPTIONS

Which option? /STEP\_AND\_MAP/: ?

EQUILIBRIUM_CALCUL	NEW_COMPOSITION_SET	SHOW_FOR_T=
GLOBAL_MINIMIZATION	OUTPUT_FILE_FOR_SHOW	STABILITY_CHECK
IGNORE_COMPOSI_SET_ORDER	PARAEQUILIBRIUM	STEP_AND_MAP
LIST_PHASE_ADDITION	PHASE_ADDITION	T-ZERO TEMPERATURE
MAJOR_CONSTITUENTS	PRESENT_PHASE	TOGGLE_ALTERNATE_MODE

Which option? /STEP\_AND\_MAP/: present

Phase name /NONE/: liquid

POLY\_3:

POLY\_3: save tcex19a1 y

... the command in full is SAVE\_WORKSPACES

POLY\_3: map

Version R mapping is selected

Organizing start points

NO INITIAL EQUILIBRIUM ADDED, TRYING TO FIX ONE

Generating start point 1

Generating start point 2

Phase region boundary 1 at: 8.426E-02 2.500E-01 1.182E+03

LIQUID

\*\* BCC\_B2

\*\* DIAMOND\_A4

\*\*\* Buffer saved on file:

c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19a\tce

x19a1.POLY3

CALCULATED 35 EQUILIBRIA

Phase region boundary 2 at: 4.045E-01 1.269E-01 9.785E+02

LIQUID

ALCU\_EPSILON

\*\* BCC\_B2

\*\* DIAMOND\_A4

SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary 2 at: 4.045E-01 1.269E-01 9.785E+02

LIQUID

\*\* ALCU\_EPSILON

\*\* BCC\_B2

Terminating at diagram limit

CALCULATED 18 EQUILIBRIA

Phase region boundary 2 at: 4.045E-01 1.269E-01 9.785E+02

LIQUID

\*\* ALCU\_EPSILON

\*\* DIAMOND\_A4

CALCULATED 20 EQUILIBRIA

Phase region boundary 2 at: 5.755E-01 8.764E-02 8.678E+02

LIQUID

\*\* ALCU\_EPSILON

ALCU\_ETA

\*\* DIAMOND\_A4

SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary 2 at: 5.755E-01 8.764E-02 8.678E+02

LIQUID

\*\* ALCU\_EPSILON

\*\* ALCU\_ETA

Terminating at diagram limit

CALCULATED 16 EQUILIBRIA

Phase region boundary 2 at: 5.755E-01 8.764E-02 8.678E+02

LIQUID

\*\* ALCU\_ETA

\*\* DIAMOND\_A4

CALCULATED 8 EQUILIBRIA

Phase region boundary 2 at: 6.299E-01 7.685E-02 8.291E+02

LIQUID

\*\* ALCU\_ETA

ALCU\_THETA

\*\* DIAMOND\_A4

SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary 2 at: 6.299E-01 7.685E-02 8.291E+02

LIQUID

\*\* ALCU\_ETA

\*\* ALCU\_THETA

Terminating at diagram limit

CALCULATED 13 EQUILIBRIA

```

Phase region boundary 2 at: 6.299E-01 7.685E-02 8.291E+02
LIQUID
** ALCU_THETA
** DIAMOND_A4
CALCULATED 18 EQUILIBRIA

Phase region boundary 2 at: 7.774E-01 7.282E-02 7.852E+02
LIQUID
** ALCU_THETA
** DIAMOND_A4
FCC_A1
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary 2 at: 7.774E-01 7.282E-02 7.852E+02
LIQUID
** ALCU_THETA
** FCC_A1
Terminating at diagram limit
CALCULATED 12 EQUILIBRIA

Phase region boundary 2 at: 7.774E-01 7.282E-02 7.852E+02
LIQUID
** DIAMOND_A4
** FCC_A1
*** SORRY CANNOT CONTINUE *** 4

CALCULATED 18 EQUILIBRIA

Phase region boundary 2 at: 8.426E-02 2.500E-01 1.182E+03
LIQUID
** BCC_B2
** DIAMOND_A4
CALCULATED 8 EQUILIBRIA

Phase region boundary 2 at: 3.577E-02 2.616E-01 1.025E+03
LIQUID
** BCC_B2
CU19SI6_ETA
** DIAMOND_A4
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary 2 at: 3.577E-02 2.616E-01 1.025E+03
LIQUID
** BCC_B2
** CU19SI6_ETA
Terminating at diagram limit
CALCULATED 12 EQUILIBRIA

Phase region boundary 2 at: 3.577E-02 2.616E-01 1.025E+03
LIQUID
** CU19SI6_ETA
** DIAMOND_A4
Terminating at diagram limit
CALCULATED 9 EQUILIBRIA
*** LAST BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19A\tce
x19a1.POLY3
CPU time for mapping 1 seconds
POLY_3:
POLY_3: @@ The monovariant line FCC/BCC/LIQ in the Cu corner is not connected,
POLY_3: @@ so add a start point for that. This is different from a MAP with
POLY_3: @@ two axes, where all connected or non-connected lines can be found
POLY_3: @@ automatically.
POLY_3: read tcex19a1
... the command in full is READ_WORKSPACES
POLY_3:
POLY_3: s-c x(al)=.1 x(si)=.1
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 16220 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY_3: adva
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liquid
POLY_3:
POLY_3: map
Version R mapping is selected

Organizing start points

NO INITIAL EQUILIBRIUM ADDED, TRYING TO FIX ONE
Generating start point 1
Generating start point 2

Phase region boundary 1 at: 4.390E-02 1.000E-01 1.285E+03
LIQUID
** BCC_B2
** FCC_A1
Terminating at diagram limit
CALCULATED 18 EQUILIBRIA

Phase region boundary 2 at: 4.390E-02 1.000E-01 1.285E+03
LIQUID
** BCC_B2
** FCC_A1
Terminating at diagram limit
CALCULATED 9 EQUILIBRIA
*** LAST BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19A\tce
x19a1.POLY3
CPU time for mapping 0 seconds
POLY_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: @@ we want the liquid compositions only
POST: s-d-a x x(liquid,al)

```

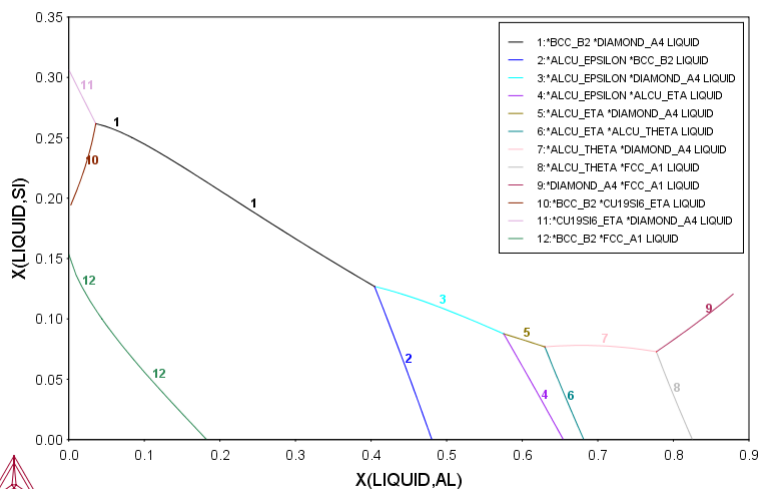
```

... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y x(liquid,si)
... the command in full is SET_DIAGRAM_AXIS
POST: s-lab b
... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: set-title example 19Aa
POST: plot
... the command in full is PLOT DIAGRAM

```

example 19Aa

2016.05.16.13.40.15  
USER: AL, CU, SI  
P=1.01325E5, N=1.



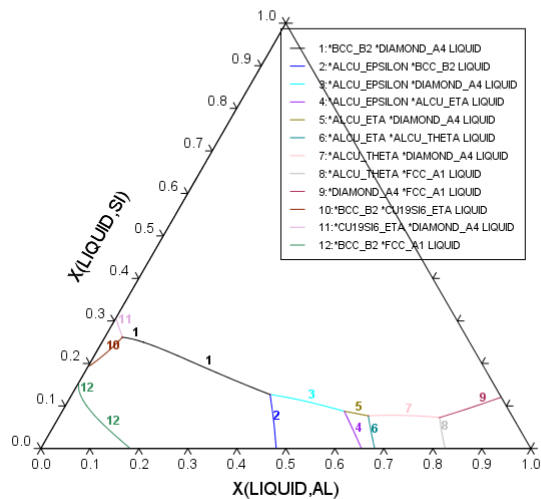
```

POST:
POST: Hit RETURN to continue
POST: @@ Make it triangular and scale the axis
POST: s-d-t
... the command in full is SET_DIAGRAM_TYPE
TRIANGULAR DIAGRAM (Y OR N) /N/: y,,,,,,
POST: s-sc y n 0 1
... the command in full is SET_SCALING_STATUS
POST: s-sc x n 0 1
... the command in full is SET_SCALING_STATUS
POST: @@ Plot the phases stable along the lines
POST: s-lab b
... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: plot
... the command in full is PLOT DIAGRAM

```

example 19Aa

2016.05.16.13.40.15  
USER: AL, CU, SI  
P=1.01325E5, N=1.



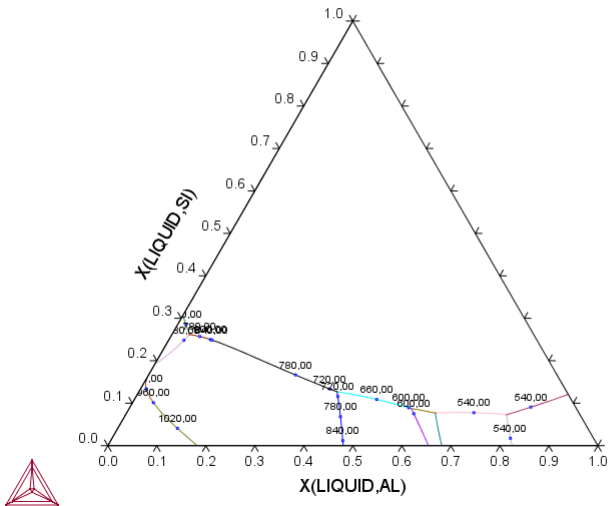
```

POST:
POST: Hit RETURN to continue
POST: @@ Take away the phase labels and add
POST: @@ tic marks along the lines (the Z axis)
POST: s-lab n
... the command in full is SET_LABEL_CURVE_OPTION
POST: s-d-a z t-c
... the command in full is SET_DIAGRAM_AXIS
POST: s-sc z n 500 1000
... the command in full is SET_SCALING_STATUS
POST: set-title example 19Ab
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

# example 19Ab

2016.05.16.13.40.15  
USER: AL, CU, SI  
P=1.01325E5, N=1.



```
POST:
POST:Hit RETURN to continue
POST: @@ We will make a new calculation to overlay these monovariant lines
POST: @@ with isothermal calculations
POST:
POST: make tcex19a y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: back
POLY_3: read tcex19a1
... the command in full is READ_WORKSPACES
POLY_3:
POLY_3: s-a-v 3
... the command in full is SET_AXIS_VARIABLE
Condition /T/: none
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 16220 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY_3: save tcex19a2 y
... the command in full is SAVE_WORKSPACES
POLY_3: l-c
... the command in full is LIST_CONDITIONS
T=1300, P=1.01325E5, N=1, X(SI)=0.25, X(AL)=0.2
DEGREES OF FREEDOM 0
POLY_3: s-c x(al)
... the command in full is SET_CONDITION
Value /.2/: .10
POLY_3: @@ One must use ADD to have several start points at different temperatures.
POLY_3: @@ But do not use default direction as that will create a lot of start points.
POLY_3: @@ Increasing the Si content will most certainly make a solid phase stable.
POLY_3: adva
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liquid
POLY_3: add 2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add -2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: @@ One may have initial equilibria for several different
POLY_3: @@ conditions at the same time. Just the axis variables have
POLY_3: @@ to be the same
POLY_3: @@ To make nice isothermal curves is not easy, one has to try
POLY_3: @@ with several start points to find all curve sections.
POLY_3: s-c t
... the command in full is SET_CONDITION
Value /1300/: 1200
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 16220 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY_3: adva
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liquid
POLY_3: add 2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add -2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: s-c t
... the command in full is SET_CONDITION
Value /1200/: 1100
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 16220 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY_3: adva
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liquid
POLY_3: add 2
```



```

... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add -2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3:
POLY_3: @@ This line exists only in Al rich corner
POLY_3: s-c x(al)=.5 x(si)=.1
... the command in full is SET_CONDITION
POLY_3: s-c t
... the command in full is SET_CONDITION
Value /1100/: 1000
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      16220 grid points in      0 s
Found the set of lowest grid points in      0 s
Calculated POLY solution      1 s, total time      1 s
POLY_3: adva
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liquid
POLY_3: add 2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add -2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3:
POLY_3: @@ A start point in the low melting Al corner too
POLY_3: s-c x(al)=.9 x(si)=.01 t=900
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      16220 grid points in      0 s
Found the set of lowest grid points in      0 s
Calculated POLY solution      0 s, total time      0 s
POLY_3: adva
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liquid
POLY_3: add 1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add -1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3:
POLY_3: map
Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point  1
Generating start point  2
Generating start point  3
Generating start point  4
Generating start point  5
Generating start point  6
Generating start point  7
Generating start point  8
Generating start point  9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard

Phase region boundary  1 at:  5.000E-02  6.891E-01
LIQUID
** DIAMOND_A4
Calculated              10 equilibria

Phase region boundary  2 at:  5.000E-02  6.891E-01
LIQUID
** DIAMOND_A4
Calculated              52 equilibria

Phase region boundary  3 at:  1.004E-01  3.055E-02
LIQUID
** FCC_A1
Calculated              21 equilibria

Phase region boundary  4 at:  1.004E-01  3.055E-02
LIQUID
** FCC_A1
Calculated              5 equilibria

Phase region boundary  5 at:  1.373E-01  1.932E-02
LIQUID
** BCC_B2
** FCC_A1

Phase region boundary  6 at:  1.463E-01  2.848E-02
LIQUID
** BCC_B2
Calculated              51 equilibria

Phase region boundary  7 at:  1.373E-01  1.932E-02
LIQUID
** FCC_A1
Calculated              27 equilibria

Phase region boundary  8 at:  5.000E-02  6.515E-01
LIQUID
** DIAMOND_A4

```

Calculated	43	equilibria
Phase region boundary 9 at:	5.000E-02	6.515E-01
LIQUID		
** DIAMOND_A4		
Calculated	52	equilibria
Phase region boundary 10 at:	1.081E-01	1.639E-01
LIQUID		
** BCC_B2		
Calculated.	16	equilibria
Phase region boundary 11 at:	2.872E-02	1.169E-01
LIQUID		
** BCC_B2		
** FCC_A1		
Phase region boundary 12 at:	2.764E-02	9.624E-02
LIQUID		
** FCC_A1		
Calculated	13	equilibria
Phase region boundary 13 at:	2.872E-02	1.169E-01
LIQUID		
** BCC_B2		
Calculated	70	equilibria
Phase region boundary 14 at:	1.081E-01	1.639E-01
LIQUID		
** BCC_B2		
Calculated	44	equilibria
Phase region boundary 15 at:	5.000E-02	6.262E-01
LIQUID		
** DIAMOND_A4		
Calculated	38	equilibria
Phase region boundary 16 at:	5.000E-02	6.262E-01
LIQUID		
** DIAMOND_A4		
Calculated	56	equilibria
Phase region boundary 17 at:	1.116E-01	1.999E-01
LIQUID		
** BCC_B2		
Calculated	23	equilibria
Phase region boundary 18 at:	1.116E-01	1.999E-01
LIQUID		
** BCC_B2		
Calculated.	34	equilibria
Phase region boundary 19 at:	4.370E-01	1.765E-02
LIQUID		
** ALCU_EPSILON		
** BCC_B2		
Phase region boundary 20 at:	4.453E-01	1.265E-02
LIQUID		
** ALCU_EPSILON		
Calculated	18	equilibria
Phase region boundary 21 at:	4.370E-01	1.765E-02
LIQUID		
** BCC_B2		
Calculated.	43	equilibria
Phase region boundary 22 at:	2.106E-02	1.939E-01
LIQUID		
** BCC_B2		
** CU19SI6_ETA		
Phase region boundary 23 at:	7.190E-03	2.263E-01
LIQUID		
** CU19SI6_ETA		
Calculated	24	equilibria
Phase region boundary 24 at:	2.500E-01	5.691E-01
LIQUID		
** DIAMOND_A4		
Calculated.	8	equilibria
Phase region boundary 25 at:	1.890E-01	5.683E-01
LIQUID		
** BCC_B2		
** DIAMOND_A4		
Phase region boundary 26 at:	3.667E-01	1.003E-01
LIQUID		
** BCC_B2		
Calculated.	5	equilibria
Phase region boundary 27 at:	3.979E-01	7.953E-02
LIQUID		
** ALCU_EPSILON		
** BCC_B2		
Phase region boundary 28 at:	4.219E-01	5.542E-02
LIQUID		
** ALCU_EPSILON		
Calculated	28	equilibria
Phase region boundary 29 at:	1.890E-01	5.683E-01
LIQUID		
** DIAMOND_A4		
Calculated	42	equilibria
Phase region boundary 30 at:	2.500E-01	5.691E-01
LIQUID		
** DIAMOND_A4		
Calculated	49	equilibria
Phase region boundary 31 at:	4.698E-01	3.348E-02
LIQUID		
** ALCU_EPSILON		
Calculated.	6	equilibria

Terminating at known equilibrium

Phase region boundary 32 at: 4.698E-01 3.348E-02

LIQUID

\*\* ALCU\_EPSILON

Calculated 27 equilibria

Phase region boundary 33 at: 9.694E-01 5.516E-03

LIQUID

\*\* FCC\_A1

Calculated 12 equilibria

Phase region boundary 34 at: 9.694E-01 5.516E-03

LIQUID

\*\* FCC\_A1

Calculated 16 equilibria

Phase region boundary 35 at: 5.506E-01 5.000E-03

LIQUID

\*\* ALCU\_EPSILON

Calculated 18 equilibria

Phase region boundary 36 at: 5.506E-01 5.000E-03

LIQUID

\*\* ALCU\_EPSILON

Calculated. 10 equilibria

Phase region boundary 37 at: 4.954E-01 4.888E-02

LIQUID

\*\* ALCU\_EPSILON

\*\* DIAMOND\_A4

Phase region boundary 38 at: 2.690E-01 5.489E-01

LIQUID

\*\* DIAMOND\_A4

Calculated 35 equilibria

Phase region boundary 39 at: 4.954E-01 4.888E-02

LIQUID

\*\* ALCU\_EPSILON

Calculated 22 equilibria

\*\*\* BUFFER SAVED ON FILE:

c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19A\tce

x19a2.POLY3

CPU time for mapping 7 seconds

POLY\_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-d-a x x(liquid,al)

... the command in full is SET\_DIAGRAM\_AXIS

POST: s-d-a y x(liquid,si)

... the command in full is SET\_DIAGRAM\_AXIS

POST: s-d-ty y,,,,

... the command in full is SET\_DIAGRAM\_TYPE

POST:

POST:

POST: set-title example 19Ac

POST:

POST: plot

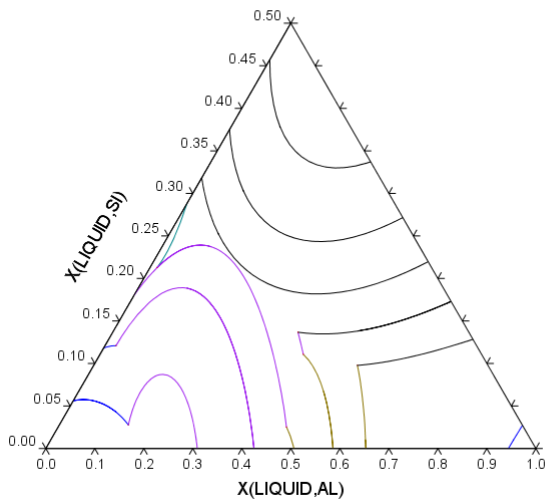
... the command in full is PLOT\_DIAGRAM

**example 19Ac**

2016.05.16.13.40.26

USER: AL, CU, SI

T=1300, P=1.01325E5, N=1



POST:

POST:Hit RETURN to continue

POST: a-e-d y tcex19a

... the command in full is APPEND\_EXPERIMENTAL\_DATA

PROLOGUE NUMBER: /0/: 0

DATASET NUMBER(s): /-1/: 1

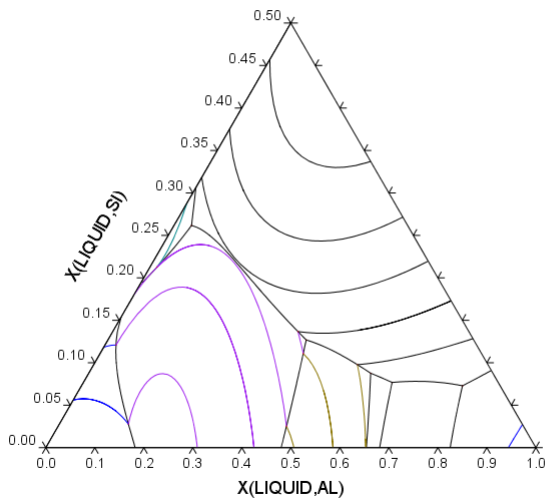
POST: set-title example 19Ad

POST:

POST: plot

... the command in full is PLOT\_DIAGRAM

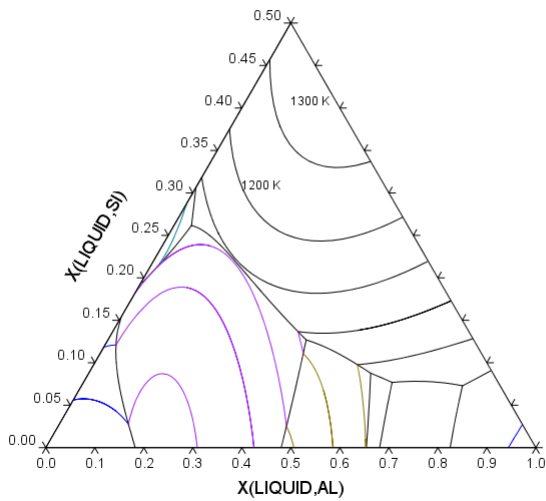
2016.05.16.13.40.26  
 USER: AL, CU, SI  
 T=1300, P=1.01325E5, N=1



```

POST:
POST:Hit RETURN to continue
POST: add .1 .4 n 1300 K
... the command in full is ADD_LABEL_TEXT
Text size: /.36/:
POST:
POST: add .1 .3 n 1200 K
... the command in full is ADD_LABEL_TEXT
Text size: /.36/:
POST:
POST: set-title example 19Ae
POST:
POST: plot
... the command in full is PLOT DIAGRAM
  
```

2016.05.16.13.40.27  
 USER: AL, CU, SI  
 T=1300, P=1.01325E5, N=1



```

POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:
  
```

## tcex19B

```
AboutSYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\tcex19B.TCM" set-echo
SYS: @@
SYS: @@
SYS: @@ Mapping of univariant equilibria with the liquid in Al-Cu-Si
SYS: @@ Part B: using TERNARY module
SYS: @@
SYS: @@ Using TERNARY module, one can easily obtain the information on
SYS: @@ invariant reactions, such as temperature and compositions.
SYS: @@
SYS: set-log ex19b,,
SYS: go ter
... the command in full is GOTO_MODULE

Quick ternary phase diagram calculation module

THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
L12_FCC B2_BCC B2_VACANCY
HIGH_SIGMA DICTRA_FCC_A1 REJECTED
Current database: Iron Demo Database

VA /- DEFINED
Database: /FEDEMO/: user tcex19_cost2.TDB
Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

VA /- DEFINED
First element: al cu si
Phase Diagram, Monovariants, or Liquidus Surface: /Phase_Diagram/: L
Min temperature, C /25/: 25
Max temperature, C /2500/: 2500
Temperature interval /100/: 100
Global minimization on: /N/: N
VA /- DEFINED
REINITIATING GES5 .....
AL CU SI
DEFINED
*** GAS INPUT IGNORED

*****
* WARNING: This database has no list of assessed systems *
* The diagram may be wrong. *
*****

Quit? /Y/: N
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
Reference REF1 missing close to line 641
Reference REF1 missing close to line 643
Reference REF1 missing close to line 645
FUNCTIONS .....

List of references for assessed data

'COST2 - TCOST507 Light Alloys Database (Version 2.1), provided by TCSAB,
1999/2003. '
-OK-
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
Forcing automatic start values
Automatic start values will be set
T = 1673.15 K
Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2

Phase region boundary 1 at: 7.327E-03 9.853E-01
LIQUID
** DIAMOND_A4
Calculated 15 equilibria

Phase region boundary 2 at: 7.327E-03 9.853E-01
LIQUID
** DIAMOND_A4
Calculated 15 equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\MON
OVAR.POLY3
CPU time for mapping 0 seconds
T = 1573.15 K

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2

Phase region boundary 1 at: 7.453E-02 8.883E-01
LIQUID
```

```

** DIAMOND_A4
Calculated                23  equilibria

Phase region boundary  2 at:  7.453E-02  8.883E-01
LIQUID
** DIAMOND_A4
Calculated                25  equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\MON
OVAR.POLY3
CPU time for mapping                0  seconds
T = 1473.15 K

```

This file contains results from a previous STEP or MAP command.  
The SAVE command will save the current status of the program but destroy  
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

```

Generating start point  1
Generating start point  2

Phase region boundary  1 at:  1.372E-01  7.942E-01
LIQUID
** DIAMOND_A4
Calculated                30  equilibria

Phase region boundary  2 at:  1.372E-01  7.942E-01
LIQUID
** DIAMOND_A4
Calculated                22  equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\MON
OVAR.POLY3
CPU time for mapping                1  seconds
T = 1373.15 K

```

This file contains results from a previous STEP or MAP command.  
The SAVE command will save the current status of the program but destroy  
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

```

Generating start point  1
Generating start point  2

Phase region boundary  1 at:  1.926E-01  7.111E-01
LIQUID
** DIAMOND_A4
Calculated                28  equilibria

Phase region boundary  2 at:  1.926E-01  7.111E-01
LIQUID
** DIAMOND_A4
Calculated                32  equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\MON
OVAR.POLY3
CPU time for mapping                0  seconds
T = 1273.15 K

```

This file contains results from a previous STEP or MAP command.  
The SAVE command will save the current status of the program but destroy  
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

```

Generating start point  1
Generating start point  2

Phase region boundary  1 at:  6.652E-01  9.329E-03
LIQUID
** BCC_B2
Calculated.                2  equilibria

Phase region boundary  2 at:  6.645E-01  6.795E-03
LIQUID
** BCC_B2
** GAMMA_H

Phase region boundary  3 at:  6.653E-01  4.077E-03
LIQUID
** GAMMA_H
Calculated                12  equilibria

Phase region boundary  4 at:  6.645E-01  6.795E-03
LIQUID
** BCC_B2
Calculated.                29  equilibria

Phase region boundary  5 at:  8.419E-01  6.666E-02
LIQUID
** BCC_B2
** FCC_A1

Phase region boundary  6 at:  8.633E-01  4.917E-02
LIQUID
** FCC_A1
Calculated                25  equilibria

Phase region boundary  7 at:  6.652E-01  9.329E-03
LIQUID
** BCC_B2
Calculated.                30  equilibria

```

Terminating at known equilibrium  
\*\*\* BUFFER SAVED ON FILE:  
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\MON  
OVAR.POLY3  
CPU time for mapping 0 seconds

This file contains results from a previous STEP or MAP command.  
The SAVE command will save the current status of the program but destroy  
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1  
Generating start point 2

Phase region boundary 1 at: 2.311E-01 6.535E-01  
LIQUID  
\*\* DIAMOND\_A4  
Calculated 34 equilibria

Phase region boundary 2 at: 2.311E-01 6.535E-01  
LIQUID  
\*\* DIAMOND\_A4  
Calculated 34 equilibria

\*\*\* BUFFER SAVED ON FILE:  
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\MON  
OVAR.POLY3  
CPU time for mapping 0 seconds  
T = 1173.15 K

This file contains results from a previous STEP or MAP command.  
The SAVE command will save the current status of the program but destroy  
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1  
Generating start point 2

Phase region boundary 1 at: 5.840E-01 7.591E-03  
LIQUID  
\*\* BCC\_B2  
Calculated 9 equilibria

Phase region boundary 2 at: 5.840E-01 7.591E-03  
LIQUID  
\*\* BCC\_B2  
Calculated. 39 equilibria

Phase region boundary 3 at: 8.543E-01 1.296E-01  
LIQUID  
\*\* BCC\_B2  
\*\* FCC\_A1

Phase region boundary 4 at: 8.749E-01 1.099E-01  
LIQUID  
\*\* FCC\_A1  
Calculated 24 equilibria

Phase region boundary 5 at: 8.543E-01 1.296E-01  
LIQUID  
\*\* BCC\_B2  
Calculated 54 equilibria  
\*\*\* BUFFER SAVED ON FILE:  
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\MON  
OVAR.POLY3  
CPU time for mapping 1 seconds

This file contains results from a previous STEP or MAP command.  
The SAVE command will save the current status of the program but destroy  
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1  
Generating start point 2

Phase region boundary 1 at: 2.562E-01 6.158E-01  
LIQUID  
\*\* DIAMOND\_A4  
Calculated 39 equilibria

Phase region boundary 2 at: 2.562E-01 6.158E-01  
LIQUID  
\*\* DIAMOND\_A4  
Calculated 37 equilibria

\*\*\* BUFFER SAVED ON FILE:  
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\MON  
OVAR.POLY3  
CPU time for mapping 0 seconds  
T = 1073.15 K

This file contains results from a previous STEP or MAP command.  
The SAVE command will save the current status of the program but destroy  
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1  
Generating start point 2

```

Phase region boundary 1 at: 5.198E-01 5.412E-03
LIQUID
** ALCU_EPSILON
Calculated 11 equilibria

Phase region boundary 2 at: 5.198E-01 5.412E-03
LIQUID
** ALCU_EPSILON
Calculated. 5 equilibria

Phase region boundary 3 at: 5.361E-01 2.533E-02
LIQUID
** ALCU_EPSILON
** BCC_B2

Phase region boundary 4 at: 5.383E-01 3.569E-02
LIQUID
** BCC_B2
Calculated. 12 equilibria

Phase region boundary 5 at: 5.962E-01 1.431E-01
LIQUID
** BCC_B2
** DIAMOND_A4

Phase region boundary 6 at: 2.789E-01 5.911E-01
LIQUID
** DIAMOND_A4
Calculated 41 equilibria

Phase region boundary 7 at: 5.361E-01 2.533E-02
LIQUID
** ALCU_EPSILON
Calculated 16 equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\MON
OVAR.POLY3
CPU time for mapping 1 seconds

```

This file contains results from a previous STEP or MAP command.  
The SAVE command will save the current status of the program but destroy  
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

```

Generating start point 1
Generating start point 2

Phase region boundary 1 at: 7.337E-01 2.597E-01
LIQUID
** CU19SI6_ETA
Calculated. 4 equilibria

Phase region boundary 2 at: 7.478E-01 2.387E-01
LIQUID
** BCC_B2
** CU19SI6_ETA

Phase region boundary 3 at: 7.525E-01 2.105E-01
LIQUID
** BCC_B2
Calculated. 8 equilibria

Phase region boundary 4 at: 6.917E-01 2.112E-01
LIQUID
** BCC_B2
** DIAMOND_A4

Phase region boundary 5 at: 3.329E-01 6.250E-01
LIQUID
** DIAMOND_A4
Calculated. 14 equilibria

Phase region boundary 6 at: 3.469E-01 6.529E-01
LIQUID
** CU19SI6_ETA
** DIAMOND_A4

Phase region boundary 7 at: 7.269E-01 2.729E-01
LIQUID
** CU19SI6_ETA
Calculated. 6 equilibria
Terminating at known equilibrium

Phase region boundary 8 at: 7.337E-01 2.597E-01
LIQUID
** CU19SI6_ETA
Calculated. 3 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\MON
OVAR.POLY3
CPU time for mapping 0 seconds
T = 973.15 K

```

This file contains results from a previous STEP or MAP command.  
The SAVE command will save the current status of the program but destroy  
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

```

Generating start point 1
Generating start point 2

Phase region boundary 1 at: 4.736E-01 5.113E-03
LIQUID
** ALCU_EPSILON

```



```

Calculated                12  equilibria

Phase region boundary  2 at:  4.736E-01  5.113E-03
  LIQUID
  ** ALCU_EPSILON
Calculated.                11  equilibria

Phase region boundary  3 at:  5.106E-01  6.209E-02
  LIQUID
  ** ALCU_EPSILON
  ** DIAMOND_A4

Phase region boundary  4 at:  2.273E-01  5.621E-01
  LIQUID
  ** DIAMOND_A4
Calculated                36  equilibria

Phase region boundary  5 at:  5.106E-01  6.209E-02
  LIQUID
  ** ALCU_EPSILON
Calculated                24  equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\MON
OVAR.POLY3
CPU time for mapping                0  seconds
T = 873.15 K

```

This file contains results from a previous STEP or MAP command.  
The SAVE command will save the current status of the program but destroy  
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

```

Generating start point  1
Generating start point  2

Phase region boundary  1 at:  3.646E-02  1.803E-02
  LIQUID
  ** FCC_A1
Calculated                15  equilibria

Phase region boundary  2 at:  3.646E-02  1.803E-02
  LIQUID
  ** FCC_A1
Calculated                33  equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\MON
OVAR.POLY3
CPU time for mapping                0  seconds

```

This file contains results from a previous STEP or MAP command.  
The SAVE command will save the current status of the program but destroy  
the results from the previous STEP or MAP commands.

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

```

Generating start point  1
Generating start point  2

Phase region boundary  1 at:  4.151E-01  5.493E-03
  LIQUID
  ** ALCU_ETA
Calculated                8  equilibria

Phase region boundary  2 at:  4.151E-01  5.493E-03
  LIQUID
  ** ALCU_ETA
Calculated.                6  equilibria

Phase region boundary  3 at:  4.241E-01  3.756E-02
  LIQUID
  ** ALCU_EPSILON
  ** ALCU_ETA

Phase region boundary  4 at:  4.398E-01  3.756E-02
  LIQUID
  ** ALCU_EPSILON
Calculated.                2  equilibria

Phase region boundary  5 at:  4.420E-01  4.464E-02
  LIQUID
  ** ALCU_EPSILON
  ** DIAMOND_A4

Phase region boundary  6 at:  1.706E-01  5.446E-01
  LIQUID
  ** DIAMOND_A4
Calculated                27  equilibria

Phase region boundary  7 at:  4.241E-01  3.756E-02
  LIQUID
  ** ALCU_ETA
Calculated                17  equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\MON
OVAR.POLY3
CPU time for mapping                0  seconds
T = 773.15 K

```

This file contains results from a previous STEP or MAP command.  
The SAVE command will save the current status of the program but destroy  
the results from the previous STEP or MAP commands.

T = 1773.15 K

Version R mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1  
Generating start point 2

Phase region boundary 1 at: 3.379E-01 7.512E-02 8.731E+02  
LIQUID  
\*\* ALCU\_EPSILON  
\*\* ALCU\_ETA  
CALCULATED 4 EQUILIBRIA

Phase region boundary 2 at: 3.369E-01 8.764E-02 8.678E+02  
LIQUID  
\*\* ALCU\_EPSILON  
\*\* ALCU\_ETA  
DIAMOND\_A4  
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary 2 at: 3.369E-01 8.764E-02 8.678E+02  
LIQUID  
\*\* ALCU\_EPSILON  
\*\* DIAMOND\_A4  
CALCULATED 25 EQUILIBRIA

Phase region boundary 2 at: 4.686E-01 1.269E-01 9.785E+02  
LIQUID  
\*\* ALCU\_EPSILON  
BCC\_B2  
\*\* DIAMOND\_A4  
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary 2 at: 4.686E-01 1.269E-01 9.785E+02  
LIQUID  
\*\* ALCU\_EPSILON  
\*\* BCC\_B2  
Terminating at diagram limit  
CALCULATED 34 EQUILIBRIA

Phase region boundary 2 at: 4.686E-01 1.269E-01 9.785E+02  
LIQUID  
\*\* BCC\_B2  
\*\* DIAMOND\_A4  
CALCULATED 43 EQUILIBRIA

Phase region boundary 2 at: 7.026E-01 2.616E-01 1.025E+03  
LIQUID  
\*\* BCC\_B2  
CU19SI6\_ETA  
\*\* DIAMOND\_A4  
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary 2 at: 7.026E-01 2.616E-01 1.025E+03  
LIQUID  
\*\* BCC\_B2  
\*\* CU19SI6\_ETA  
Terminating at known equilibrium  
CALCULATED 37 EQUILIBRIA

Phase region boundary 2 at: 7.026E-01 2.616E-01 1.025E+03  
LIQUID  
\*\* CU19SI6\_ETA  
\*\* DIAMOND\_A4  
\*\*\* SORRY CANNOT CONTINUE \*\*\* 4  
CALCULATED 16 EQUILIBRIA

Phase region boundary 2 at: 3.369E-01 8.764E-02 8.678E+02  
LIQUID  
\*\* ALCU\_ETA  
\*\* DIAMOND\_A4  
CALCULATED 9 EQUILIBRIA

Phase region boundary 2 at: 2.933E-01 7.685E-02 8.291E+02  
LIQUID  
\*\* ALCU\_ETA  
ALCU\_THETA  
\*\* DIAMOND\_A4  
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary 2 at: 2.933E-01 7.685E-02 8.291E+02  
LIQUID  
\*\* ALCU\_ETA  
\*\* ALCU\_THETA  
Terminating at diagram limit  
CALCULATED 14 EQUILIBRIA

Phase region boundary 2 at: 2.933E-01 7.685E-02 8.291E+02  
LIQUID  
\*\* ALCU\_THETA  
\*\* DIAMOND\_A4  
CALCULATED 17 EQUILIBRIA

Phase region boundary 2 at: 1.498E-01 7.282E-02 7.852E+02  
LIQUID  
\*\* ALCU\_THETA  
\*\* DIAMOND\_A4  
FCC\_A1  
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary 2 at: 1.498E-01 7.282E-02 7.852E+02  
LIQUID  
\*\* ALCU\_THETA  
\*\* FCC\_A1  
Terminating at diagram limit  
CALCULATED 12 EQUILIBRIA

Phase region boundary 2 at: 1.498E-01 7.282E-02 7.852E+02  
LIQUID  
\*\* DIAMOND\_A4  
\*\* FCC\_A1  
Terminating at diagram limit  
CALCULATED 21 EQUILIBRIA

Phase region boundary 2 at: 3.379E-01 7.512E-02 8.731E+02  
LIQUID  
\*\* ALCU\_EPSILON



\*\*\* SORRY CANNOT CONTINUE \*\*\* 9

CALCULATED 46 EQUILIBRIA

Phase region boundary 2 at: 8.482E-01 6.736E-02 1.273E+03

LIQUID

\*\* BCC\_B2

\*\* FCC\_A1

Terminating at diagram limit

CALCULATED 13 EQUILIBRIA

Phase region boundary 2 at: 6.503E-01 8.154E-03 1.273E+03

LIQUID

\*\* BCC\_B2

\*\* GAMMA\_H

Terminating at diagram limit

CALCULATED 13 EQUILIBRIA

Phase region boundary 2 at: 6.503E-01 8.154E-03 1.273E+03

LIQUID

\*\* BCC\_B2

\*\* GAMMA\_H

Terminating at diagram limit

CALCULATED 9 EQUILIBRIA

\*\*\* LAST BUFFER SAVED ON FILE:

c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\MON

OVAR.POLY3

CPU time for mapping 0 seconds

Forcing automatic start values

Automatic start values will be set

Forcing automatic start values

Automatic start values will be set

Forcing automatic start values

Automatic start values will be set

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Automatic start values will be set

Forcing automatic start values

```

    LIQUID
** BCC_B2
** FCC_A1

Phase region boundary 6 at: 8.633E-01 4.917E-02
    LIQUID
** FCC_A1
Calculated 25 equilibria

Phase region boundary 7 at: 8.633E-01 4.917E-02
    LIQUID
** FCC_A1
Calculated 25 equilibria

Phase region boundary 8 at: 6.645E-01 6.795E-03
    LIQUID
** BCC_B2
Calculated. 26 equilibria
Terminating at known equilibrium

Phase region boundary 9 at: 6.653E-01 4.077E-03
    LIQUID
** GAMMA_H
Calculated 12 equilibria

Phase region boundary 10 at: 7.327E-03 9.853E-01
    LIQUID
** DIAMOND_A4
Calculated 15 equilibria

Phase region boundary 11 at: 7.327E-03 9.853E-01
    LIQUID
** DIAMOND_A4
Calculated 15 equilibria

Phase region boundary 12 at: 7.453E-02 8.883E-01
    LIQUID
** DIAMOND_A4
Calculated 23 equilibria

Phase region boundary 13 at: 7.453E-02 8.883E-01
    LIQUID
** DIAMOND_A4
Calculated 25 equilibria

Phase region boundary 14 at: 1.372E-01 7.942E-01
    LIQUID
** DIAMOND_A4
Calculated 30 equilibria

Phase region boundary 15 at: 1.372E-01 7.942E-01
    LIQUID
** DIAMOND_A4
Calculated 22 equilibria

Phase region boundary 16 at: 1.926E-01 7.111E-01
    LIQUID
** DIAMOND_A4
Calculated 28 equilibria

Phase region boundary 17 at: 1.926E-01 7.111E-01
    LIQUID
** DIAMOND_A4
Calculated 32 equilibria

Phase region boundary 18 at: 6.652E-01 9.329E-03
    LIQUID
** BCC_B2
Calculated. 2 equilibria
Terminating at known equilibrium

Phase region boundary 19 at: 6.652E-01 9.329E-03
    LIQUID
** BCC_B2
Calculated. 30 equilibria
Terminating at known equilibrium

Phase region boundary 20 at: 2.311E-01 6.535E-01
    LIQUID
** DIAMOND_A4
Calculated 34 equilibria

Phase region boundary 21 at: 2.311E-01 6.535E-01
    LIQUID
** DIAMOND_A4
Calculated 40 equilibria

Phase region boundary 22 at: 5.840E-01 7.591E-03
    LIQUID
** BCC_B2
Calculated 9 equilibria

Phase region boundary 23 at: 5.840E-01 7.591E-03
    LIQUID
** BCC_B2
Calculated. 39 equilibria

Phase region boundary 24 at: 8.543E-01 1.296E-01
    LIQUID
** BCC_B2
** FCC_A1

Phase region boundary 25 at: 8.749E-01 1.099E-01
    LIQUID
** FCC_A1
Calculated 24 equilibria

Phase region boundary 26 at: 8.543E-01 1.296E-01
    LIQUID
** BCC_B2
Calculated 54 equilibria

Phase region boundary 27 at: 2.562E-01 6.158E-01
    LIQUID
** DIAMOND_A4
Calculated 39 equilibria

```

Phase region boundary 28 at: 2.562E-01 6.158E-01  
LIQUID  
\*\* DIAMOND\_A4  
Calculated 37 equilibria

Phase region boundary 29 at: 5.198E-01 5.412E-03  
LIQUID  
\*\* ALCU\_EPSILON  
Calculated 11 equilibria

Phase region boundary 30 at: 5.198E-01 5.412E-03  
LIQUID  
\*\* ALCU\_EPSILON  
Calculated. 5 equilibria

Phase region boundary 31 at: 5.361E-01 2.533E-02  
LIQUID  
\*\* ALCU\_EPSILON  
\*\* BCC\_B2

Phase region boundary 32 at: 5.383E-01 3.569E-02  
LIQUID  
\*\* BCC\_B2  
Calculated. 12 equilibria

Phase region boundary 33 at: 5.962E-01 1.431E-01  
LIQUID  
\*\* BCC\_B2  
\*\* DIAMOND\_A4

Phase region boundary 34 at: 2.789E-01 5.911E-01  
LIQUID  
\*\* DIAMOND\_A4  
Calculated 41 equilibria

Phase region boundary 35 at: 5.361E-01 2.533E-02  
LIQUID  
\*\* ALCU\_EPSILON  
Calculated 16 equilibria

Phase region boundary 36 at: 7.337E-01 2.597E-01  
LIQUID  
\*\* CU19SI6\_ETA  
Calculated. 4 equilibria

Phase region boundary 37 at: 7.478E-01 2.387E-01  
LIQUID  
\*\* BCC\_B2  
\*\* CU19SI6\_ETA

Phase region boundary 38 at: 7.525E-01 2.105E-01  
LIQUID  
\*\* BCC\_B2  
Calculated. 8 equilibria

Phase region boundary 39 at: 6.917E-01 2.112E-01  
LIQUID  
\*\* BCC\_B2  
\*\* DIAMOND\_A4

Phase region boundary 40 at: 3.329E-01 6.250E-01  
LIQUID  
\*\* DIAMOND\_A4  
Calculated. 14 equilibria

Phase region boundary 41 at: 3.469E-01 6.529E-01  
LIQUID  
\*\* CU19SI6\_ETA  
\*\* DIAMOND\_A4

Phase region boundary 42 at: 7.269E-01 2.729E-01  
LIQUID  
\*\* CU19SI6\_ETA  
Calculated. 6 equilibria  
Terminating at known equilibrium

Phase region boundary 43 at: 7.337E-01 2.597E-01  
LIQUID  
\*\* CU19SI6\_ETA  
Calculated. 3 equilibria  
Terminating at known equilibrium

Phase region boundary 44 at: 4.736E-01 5.113E-03  
LIQUID  
\*\* ALCU\_EPSILON  
Calculated 12 equilibria

Phase region boundary 45 at: 4.736E-01 5.113E-03  
LIQUID  
\*\* ALCU\_EPSILON  
Calculated. 11 equilibria

Phase region boundary 46 at: 5.106E-01 6.209E-02  
LIQUID  
\*\* ALCU\_EPSILON  
\*\* DIAMOND\_A4

Phase region boundary 47 at: 2.273E-01 5.621E-01  
LIQUID  
\*\* DIAMOND\_A4  
Calculated 36 equilibria

Phase region boundary 48 at: 5.106E-01 6.209E-02  
LIQUID  
\*\* ALCU\_EPSILON  
Calculated 24 equilibria

Phase region boundary 49 at: 3.646E-02 1.803E-02  
LIQUID  
\*\* FCC\_A1  
Calculated 15 equilibria

Phase region boundary 50 at: 3.646E-02 1.803E-02  
LIQUID  
\*\* FCC\_A1

```

Calculated                      33 equilibria

Phase region boundary  51 at:    4.151E-01  5.493E-03
  LIQUID
  ** ALCU_ETA
Calculated                      8 equilibria

Phase region boundary  52 at:    4.151E-01  5.493E-03
  LIQUID
  ** ALCU_ETA
Calculated.                    6 equilibria

Phase region boundary  53 at:    4.241E-01  3.756E-02
  LIQUID
  ** ALCU_EPSILON
  ** ALCU_ETA
Phase region boundary  54 at:    4.398E-01  3.756E-02
  LIQUID
  ** ALCU_EPSILON
Calculated.                    2 equilibria

Phase region boundary  55 at:    4.420E-01  4.464E-02
  LIQUID
  ** ALCU_EPSILON
  ** DIAMOND_A4
Phase region boundary  56 at:    1.706E-01  5.446E-01
  LIQUID
  ** DIAMOND_A4
Calculated -                    27 equilibria

Phase region boundary  57 at:    4.241E-01  3.756E-02
  LIQUID
  ** ALCU_ETA
Calculated                      17 equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex19B\MON
OVAR.POLY3
CPU time for mapping              6 seconds

```

POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

INVARIANT REACTIONS:

```

E 1:  751.65 C: LIQUID -> BCC_B2 + CU19SI6 + DIAMOND
U 1:  705.34 C: LIQUID + BCC_B2 -> ALCU_EPS + DIAMOND
U 2:  594.68 C: LIQUID + ALCU_EPS -> ALCU_ETA + DIAMOND
U 3:  555.98 C: LIQUID + ALCU_ETA -> ALCU_THE + DIAMOND
E 2:  512.07 C: LIQUID -> ALCU_THE + DIAMOND + FCC_A1

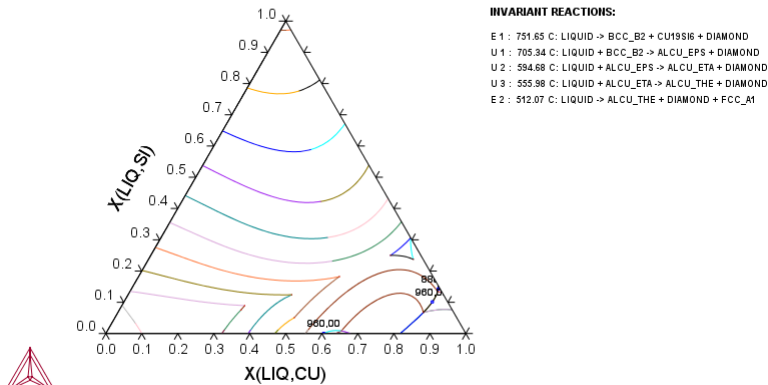
```

AL-CU-SI (600C/1400C/100C) 16 s

```

2016.05.16.13.42.56
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

```

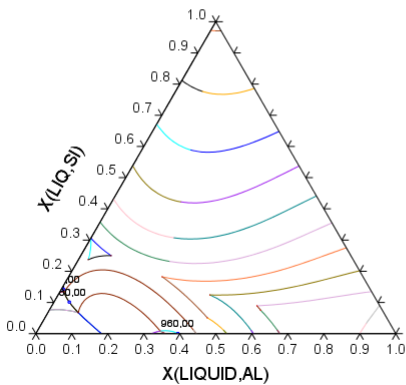
```

POST: s-d-a x x(liquid,al)
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 19B
POST: plot
... the command in full is PLOT_DIAGRAM

```

2016.05.16.13.42.56  
USER: AL, CU, SI  
P=1E5, N=1

example 19B



**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:



About

```
SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex20\tcex20.TCM"SYS: set-echo
SYS: @@
SYS: @@
SYS: @@ Example showing how to calculate an adiabatic decompression
SYS: @@ using the geochemical database
SYS: @@
SYS: set-log ex20,,
SYS: go da
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
LI2_FCC          B2_BCC          B2_VACANCY
HIGH SIGMA      DICTRA_FCC_A1   REJECTED
TDB_TCFE8: sw user PGE0.TDB
... the command in full is SWITCH_DATABASE
Current database: User defined DataBase

O              VA DEFINED
STEAM          OXYGEN          HYDROGEN
REJECTED
CARBON MONOXIDE CARBON_DIOXIDE  METHANE
REJECTED
TDB_USER: d-sys mg si
... the command in full is DEFINE_SYSTEM
MG            SI DEFINED
TDB_USER: l-sys
... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:
GAS:G          :O2:
> Gaseous Mixture with C-H-O species, using ideal gas model
A_QUARTZ       :SI1O2:
B_QUARTZ       :SI1O2:
CRISTOBALITE   :SI1O2:
TRIDYMITE      :SI1O2:
COESITE        :SI1O2:
STISHOVITE     :SI1O2:
PERICLASE      :MG1O1:
FORSTERITE     :SI1MG2O4:
BETA_FORSTERITE :SI1MG2O4:
GAMMA_FORSTERITE :SI1MG2O4:
ILMENITE MG    :SI1MG1O3:
MG_PEROVSKITE  :SI1MG1O3:
CLINOENSTATITE :SI1MG1O3:
ORTHOENSTATITE :SI1MG1O3:
PROTOENSTATITE :SI1MG1O3:
CLINOENSTHP    :SI1MG1O3:
GARNET MG      :SI1MG1O3:
TDB_USER: rej ph gas proto
... the command in full is REJECT
GAS:G          PROTOENSTATITE REJECTED
TDB_USER: get
... the command in full is GET_DATA
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....
-OK-
TDB_USER: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3: @@ We define more convenient components
POLY_3: def-com mgo o sio2
... the command in full is DEFINE_COMPONENTS
POLY_3: l-st
... the command in full is LIST_STATUS
Option /CPS/: CPS
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS  REF. STATE  T(K)          P(Pa)
VA              ENTERED SER
MGO             ENTERED SER
O               ENTERED SER
SIO2            ENTERED SER
*** STATUS FOR ALL PHASES
PHASE          STATUS  DRIVING FORCE  MOLES
TRIDYMITE      ENTERED  0.000000E+00  0.000000E+00
STISHOVITE     ENTERED  0.000000E+00  0.000000E+00
PERICLASE      ENTERED  0.000000E+00  0.000000E+00
ORTHOENSTATITE ENTERED  0.000000E+00  0.000000E+00
MG_PEROVSKITE  ENTERED  0.000000E+00  0.000000E+00
ILMENITE MG    ENTERED  0.000000E+00  0.000000E+00
GARNET MG      ENTERED  0.000000E+00  0.000000E+00
GAMMA_FORSTERITE ENTERED  0.000000E+00  0.000000E+00
FORSTERITE     ENTERED  0.000000E+00  0.000000E+00
CRISTOBALITE   ENTERED  0.000000E+00  0.000000E+00
COESITE        ENTERED  0.000000E+00  0.000000E+00
CLINOENSTHP    ENTERED  0.000000E+00  0.000000E+00
CLINOENSTATITE ENTERED  0.000000E+00  0.000000E+00
B_QUARTZ       ENTERED  0.000000E+00  0.000000E+00
BETA_FORSTERITE ENTERED  0.000000E+00  0.000000E+00
A_QUARTZ       ENTERED  0.000000E+00  0.000000E+00
*** STATUS FOR ALL SPECIES
MG              ENTERED  O              ENTERED  SI1MG1O3 ENTERED  SIO2      ENTERED
MG1O1          ENTERED  O2             ENTERED  SI1MG2O4 ENTERED  VA        ENTERED
MGO            ENTERED  SI              ENTERED  SI1O2    ENTERED
POLY_3:Hit RETURN to continue
POLY_3: @@ and specify a composition assumed to be
POLY_3: @@ present in the earth mantle
POLY_3: s-i-a n(mgo)=80
... the command in full is SET_INPUT_AMOUNTS
POLY_3: s-i-a n(silmglo3)=100
... the command in full is SET_INPUT_AMOUNTS
POLY_3: l-c
... the command in full is LIST_CONDITIONS
N(MGO)=180, N(SIO2)=100
DEGREES OF FREEDOM 3
```

```

POLY_3:Hit RETURN to continue
POLY_3: @@ There is an error if mgsio3 is used instead of the defined silmglo3,
POLY_3: @@ since mgsio3 is not defined as a species.
POLY_3: s-c t=2200,p=2e10
... the command in full is SET_CONDITION
POLY_3: save tcex20 y
... the command in full is SAVE_WORKSPACES
POLY_3: @@ We have no degree of freedom with respect
POLY_3: @@ to oxygen so set its activity to unity (or
POLY_3: @@ any positive number)
POLY_3: s-c ac(o)=1
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated      16 grid points in      0 s
    31 ITS, CPU TIME USED    0 SECONDS
POLY_3: save tcex20 y
... the command in full is SAVE_WORKSPACES
POLY_3: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE          STATUS      DRIVING FORCE    MOLES
GARNET MG      ENTERED      0.000000E+00    4.000000E+01
BETA_FORSTERITE ENTERED      0.000000E+00    2.400000E+02
GAMMA_FORSTERITE ENTERED     -5.946730E-03    0.000000E+00
MG_PEROVSKITE  ENTERED     -2.558352E-02    0.000000E+00
ILMENITE MG    ENTERED     -4.828445E-02    0.000000E+00
PERICLASE      ENTERED     -9.575143E-02    0.000000E+00
CLINOENSTHP    ENTERED     -1.541632E-01    0.000000E+00
ORTHOENSTATITE ENTERED     -2.197450E-01    0.000000E+00
CLINOENSTATITE ENTERED     -2.394369E-01    0.000000E+00
FORSTERITE     ENTERED     -2.417190E-01    0.000000E+00
STISHOVITE     ENTERED     -3.053984E-01    0.000000E+00
COESITE        ENTERED     -3.775316E+00    0.000000E+00
ENTERED PHASES WITH DRIVING FORCE LESS THAN -7.835592E+00
A QUARTZ B QUARTZ TRIDYMIT CRISTOBALITE
POLY_3: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: X
Output from POLY-3, equilibrium =      1, label A0 , database: USER

Conditions:
N(MGO)=180, N(SIO2)=100, T=2200, P=2E10, AC(O)=1
DEGREES OF FREEDOM 0

Temperature 2200.00 K ( 1926.85 C), Pressure 2.000000E+10
Number of moles of components 2.800000E+02, Mass in grams 1.32632E+04
Total Gibbs energy -1.80863E+08, Enthalpy -9.91578E+07, Volume 3.55512E-03

Component      Moles      M-Fraction Activity Potential Ref.stat
MGO             1.8000E+02    6.4286E-01 7.6674E-14 -5.5240E+05 SER
O               0.0000E+00    0.0000E+00 1.0000E+00 0.0000E+00 SER
SIO2            1.0000E+02    3.5714E-01 4.6393E-20 -8.1430E+05 SER

BETA_FORSTERITE      Status ENTERED      Driving force 0.0000E+00
Moles 2.4000E+02, Mass 1.1255E+04, Volume fraction 8.5320E-01 Mole fractions:
MGO 6.66667E-01 SIO2 3.33333E-01 O 0.00000E+00

GARNET MG           Status ENTERED      Driving force 0.0000E+00
Moles 4.0000E+01, Mass 2.0078E+03, Volume fraction 1.4680E-01 Mole fractions:
MGO 5.00000E-01 SIO2 5.00000E-01 O 0.00000E+00
POLY_3:Hit RETURN to continue
POLY_3: ent fun dens=le-3*bm/vm;
... the command in full is ENTER_SYMBOL
POLY_3: sh dens
... the command in full is SHOW_VALUE
DENS=3730.7358
POLY_3: @@ We have now found the equilibrium at this
POLY_3: @@ pressure. Now assume this system is decompressed
POLY_3: @@ adiabatically. What will the new temperature become?
POLY_3: s-c h
... the command in full is SET_CONDITION
Value /-99157833.21/:
POLY_3: s-c t
... the command in full is SET_CONDITION
Value /2200/: none
POLY_3: l-c
... the command in full is LIST_CONDITIONS
N(MGO)=180, N(SIO2)=100, P=2E10, AC(O)=1, H=-9.91578E7
DEGREES OF FREEDOM 0
POLY_3:Hit RETURN to continue
POLY_3: @@ Now t is independent, calculate the equilibrium and get t
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Using already calculated grid
    6 ITS, CPU TIME USED    0 SECONDS
POLY_3: sh t
... the command in full is SHOW_VALUE
T=2200.
POLY_3:Hit RETURN to continue
POLY_3: @@ No big surprise! the same temperature. Now change pressure
POLY_3: s-c p
... the command in full is SET_CONDITION
Value /2E+10/: 150e8
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated      16 grid points in      0 s
    18 ITS, CPU TIME USED    0 SECONDS
POLY_3: sh t
... the command in full is SHOW_VALUE
T=2977.6276
POLY_3:Hit RETURN to continue
POLY_3: @@ We will also have a new density and another set of
POLY_3: @@ stable phases.
POLY_3: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:

```

**Options /VXCS/:**

Output from POLY-3, equilibrium = 1, label A0 , database: USER

**Conditions:**

N(MGO)=180, N(SiO2)=100, P=1.5E10, AC(O)=1, H=-9.91578E7  
DEGREES OF FREEDOM 0

Temperature 2977.63 K ( 2704.48 C), Pressure 1.500000E+10  
Number of moles of components 2.80000E+02, Mass in grams 1.32632E+04  
Total Gibbs energy -2.30661E+08, Enthalpy -9.91578E+07, Volume 3.59115E-03

Component	Moles	M-Fraction	Activity	Potential	Ref.stat
MGO	1.8000E+02	6.4286E-01	4.6875E-13	-7.0283E+05	SER
O	0.0000E+00	0.0000E+00	1.0000E+00	0.0000E+00	SER
SiO2	1.0000E+02	3.5714E-01	5.3688E-19	-1.0415E+06	SER

GARNET\_MG Status ENTERED Driving force 0.0000E+00  
Moles 2.0000E+02, Mass 1.0039E+04, Volume fraction 7.4847E-01 Mole fractions:  
MGO 5.0000E-01 SiO2 5.0000E-01 O 0.0000E+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 1.0000E+00 SiO2 0.0000E+00 O 0.0000E+00

**POLY\_3:** sh dens

... the command in full is SHOW\_VALUE

DENS=3693.3029

**POLY\_3:** sh v

... the command in full is SHOW\_VALUE

V=3.5911547E-3

**POLY\_3:** sh vm

... the command in full is SHOW\_VALUE

VM=1.2825553E-5

**POLY\_3:**

**POLY\_3:** set-inter

... the command in full is SET\_INTERACTIVE

**POLY\_3:**

tcex21

About License library version: 8.5.1.0017  
Linked: Mon May 16 09:31:44 2016

```
SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex21\tcex21.TCM" set-echo
SYS: @@
SYS: @@
SYS: @@ Demonstrates the use of a user-defined database, calculate a ternary isotherm in Fe-Cr-Ni.
SYS: @@
SYS: @@
SYS: set-log ex21,,,
SYS: go da
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
L12 FCC B2_BCC B2_VACANCY
HIGH_SIGMA DICTRA_FCC_A1 REJECTED
TDB_TCFe8: sw user tcex21
... the command in full is SWITCH_DATABASE
Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

VA DEFINED
TDB_USER: def-sys *
... the command in full is DEFINE_SYSTEM
/- VA CR
FE NI DEFINED
TDB_USER: li-sys
... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:
LIQUID:L :CR FE NI:
BCC_A2 :CR FE NI:VA:
FCC_A1 :CR FE NI:VA:
HCP_A3 :CR FE NI:VA:
SIGMA :FE NI:CR:CR FE NI:
TDB_USER:Hit RETURN to continue
TDB_USER: get
... the command in full is GET_DATA
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ...

List of references for assessed data

'A.T. Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4, p 317-425; '
'J.O. Andersson, B. Sundman, Calphad 11(1987)1 p 83-92 TRITA-MAC 270
(1986); Cr-Fe'
'Byeong-Joo Lee, unpublished revision (1991); C-Cr-Fe-Ni'
'Byeong-Joo Lee, Calphad 16(1992)2, p 121-149; carbides'
'A. Dinsdale, T. Chart, MTDS NPL, unpublished work (1986); Fe-Ni'
'A. Dinsdale, T. Chart, MTDS NPL, unpublished work (1986); Cr-Ni'
'A.F. Guillermet, Z. Metallkde. 79(1988)8 p 524-536, TRITA-MAC 362 (1988);
C-Co-Ni, C-Co-Fe-Ni'
'K. Frisk, Metall. Trans. 21A (1990)9 p 2477-2488, Cr-Fe-N'
'Unassessed parameter, linear combination of unary data.'
'P. Gustafson, Calphad 12(1987)3 p 277-292, Cr-Ni-W '
-OK-
TDB_USER: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3: @@ With 3 components we must set 5 conditions
POLY_3: s-c t=1073 p=1e5 n=1 x(cr)=.2 x(ni)=.2
... the command in full is SET_CONDITION
POLY_3: l-c
... the command in full is LIST_CONDITIONS
T=1073, P=1E5, N=1, X(CR)=0.2, X(NI)=0.2
DEGREES OF FREEDOM 0
POLY_3:
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 9315 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY_3: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium = 1, label A0 , database: USER

Conditions:
T=1073, P=1E5, N=1, X(CR)=0.2, X(NI)=0.2
DEGREES OF FREEDOM 0

Temperature 1073.00 K ( 799.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 5.56454E+01
Total Gibbs energy -5.39559E+04, Enthalpy 3.01555E+04, Volume 0.00000E+00

Component Moles W-Fraction Activity Potential Ref.stat
CR 2.0000E-01 1.8688E-01 5.8626E-03 -4.5849E+04 SER
FE 6.0000E-01 6.0217E-01 3.1002E-03 -5.1533E+04 SER
NI 2.0000E-01 2.1094E-01 4.2164E-04 -6.9332E+04 SER

FCC A1 Status ENTERED Driving force 0.0000E+00
Moles 1.0000E+00, Mass 5.5645E+01, Volume fraction 0.0000E+00 Mass fractions:
FE 6.02174E-01 NI 2.10943E-01 CR 1.86883E-01
POLY_3:Hit RETURN to continue
POLY_3: @@ Define axis
POLY_3: s-a-v 1 x(cr) 0 1,,,
... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(ni) 0 1,,,
... the command in full is SET_AXIS_VARIABLE
POLY_3: save tcex21 y
... the command in full is SAVE_WORKSPACES
```

```

POLY_3: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
ERROR 1611 when calculating equilibrium
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18

Phase region boundary 1 at: 3.521E-02 1.510E-02
  BCC_A2
  ** FCC_A1
Calculated. 20 equilibria

Phase region boundary 2 at: 2.615E-01 6.190E-02
  BCC_A2
  ** FCC_A1
  ** SIGMA

Phase region boundary 3 at: 3.723E-01 3.566E-02
  BCC_A2
  ** SIGMA
Calculated 21 equilibria

Phase region boundary 4 at: 3.168E-01 6.107E-02
  FCC_A1
  ** SIGMA
Calculated. 20 equilibria

Phase region boundary 5 at: 4.140E-01 2.295E-01
  ** BCC_A2
  FCC_A1
  ** SIGMA

Phase region boundary 6 at: 5.304E-01 1.820E-01
  ** BCC_A2
  FCC_A1
Calculated 43 equilibria

Phase region boundary 7 at: 6.616E-01 7.178E-02
  ** BCC_A2
  SIGMA
Calculated 31 equilibria

Phase region boundary 8 at: 2.615E-01 6.190E-02
  BCC_A2
  ** FCC_A1
Calculated 33 equilibria

Phase region boundary 9 at: 3.521E-02 1.510E-02
  BCC_A2
  ** FCC_A1
Calculated 15 equilibria

Phase region boundary 10 at: 1.095E-02 2.044E-02
  BCC_A2
  ** FCC_A1
Calculated 18 equilibria

Phase region boundary 11 at: 1.095E-02 2.044E-02
  BCC_A2
  ** FCC_A1
Calculated. 22 equilibria
Terminating at known equilibrium

Phase region boundary 12 at: 3.838E-01 1.780E-02
  BCC_A2
  ** SIGMA
Calculated. 2 equilibria
Terminating at known equilibrium

Phase region boundary 13 at: 3.838E-01 1.780E-02
  BCC_A2
  ** SIGMA
Calculated 21 equilibria

Phase region boundary 14 at: 5.848E-01 2.838E-02
  BCC_A2
  ** SIGMA
Calculated 32 equilibria

Phase region boundary 15 at: 5.848E-01 2.838E-02
  BCC_A2
  ** SIGMA
Calculated. 8 equilibria
Terminating at known equilibrium

Phase region boundary 16 at: 5.404E-01 9.033E-03

```

```

    BCC_A2
** SIGMA
Calculated.                12 equilibria

Phase region boundary 17 at:  5.404E-01  9.033E-03
    BCC_A2
** SIGMA
Calculated.                13 equilibria
Terminating at known equilibrium

Phase region boundary 18 at:  4.123E-01  2.273E-01
    FCC_A1
** SIGMA
Calculated.                19 equilibria
Terminating at known equilibrium

Phase region boundary 19 at:  4.123E-01  2.273E-01
    FCC_A1
** SIGMA
Calculated.                2 equilibria
Terminating at known equilibrium

Phase region boundary 20 at:  9.183E-03  2.090E-02
    BCC_A2
    FCC_A1
Calculated.                13 equilibria

Phase region boundary 21 at:  9.183E-03  2.090E-02
    BCC_A2
    FCC_A1
Calculated.                22 equilibria
Terminating at known equilibrium

Phase region boundary 22 at:  6.363E-01  2.710E-01
    BCC_A2
    FCC_A1
Calculated.                16 equilibria
Terminating at known equilibrium

Phase region boundary 23 at:  6.363E-01  2.710E-01
    BCC_A2
    FCC_A1
Calculated.                26 equilibria

Phase region boundary 24 at:  6.789E-01  3.114E-01
    BCC_A2
    FCC_A1
Calculated.                22 equilibria
Terminating at known equilibrium

Phase region boundary 25 at:  6.789E-01  3.114E-01
    BCC_A2
    FCC_A1
Calculated.                16 equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex21\tcex
21.POLY3
CPU time for mapping                1 seconds
POLY_3: post

```

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

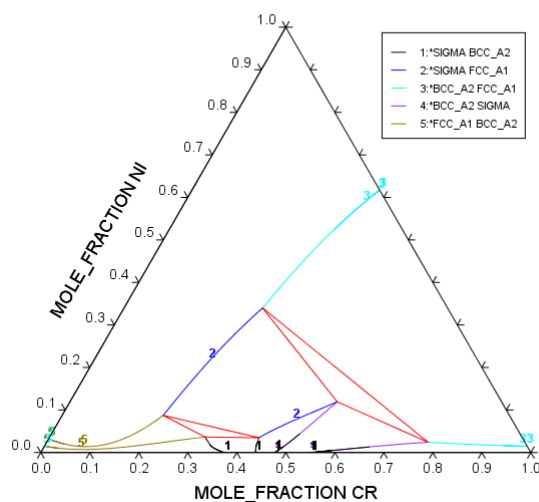
```

POST:
POST: set-title example 21a
POST: se-d-ty y,,,
... the command in full is SET_DIAGRAM_TYPE
POST: s-l b
... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
... the command in full is PLOT DIAGRAM

```

example 21a

2016.05.16.13.46.33  
 USER: CR, FE, NI  
 T=1073, P=1E5, N=1



```

POST:
POST: Hit RETURN to continue
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

```

## About

```

SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex22\tcex22.TCM" set-echo
SYS: @@
SYS: @@
SYS: @@ Calculation of a heat balance. In this case C3H8 is burned in
SYS: @@ oxygen and the adiabatic flame temperature is calculated.
SYS: @@
SYS: set-log ex22,,
SYS: go da
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
LI2_FCC B2_BCC B2_VACANCY
HIGH_SIGMA DICTRA_FCC_A1 REJECTED
TDB_TCFE8: sw ssb5
... the command in full is SWITCH_DATABASE
Current database: SGTE Substances Database v5.1

VA DEFINED
TDB_SSUB5: def-sys c o h
... the command in full is DEFINE_SYSTEM
C O H
DEFINED
TDB_SSUB5: get
... the command in full is GET_DATA
REINITIATING GES5 .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

C1<G> T.C.R.A.S. Class: 1
C1<G> C<G>
C1H1<G> T.C.R.A.S. Class: 2
C1H1<G> CH<G>
C1H1O1<G> T.C.R.A.S. Class: 4
C1H1O1<G> HCO<G>
FORMYL <GAS>
C1H1O2<G> T.C.R.A.S. Class: 6
C1H1O2<G>
C1H2<G> T.C.R.A.S. Class: 5
C1H2<G> CH2<G> METHYLENE
METHYLENE <GAS>
C1H2O1<G> T.C.R.A.S. Class: 5
C1H2O1<G> CH2O<G>
FORMALDEHYDE <GAS>
C1H2O2_CIS<G> T.C.R.A.S. Class: 5
C1H2O2_CIS<G>
C1H2O2_DIOXIRANE<G> T.C.R.A.S. Class: 6
C1H2O2_DIOXIRANE<G>
S298 corrected and cp refitted
due to corrected data in IVTAN2000 7/2002
C1H2O2_TRANS<G> T.C.R.A.S. Class: 5
C1H2O2_TRANS<G>
C1H3<G> T.C.R.A.S. Class: 5
C1H3<G> CH3<G>
METHYL, Gaseous Standard State.
C1H3O1_CH2OH<G> T.C.R.A.S. Class: 6
C1H3O1_CH2OH<G>
C1H3O1_CH3O<G> T.C.R.A.S. Class: 5
C1H3O1_CH3O<G>
C1H4<G> T.C.R.A.S. Class: 5
C1H4<G> CH4<G> METHANE
METHANE, Gaseous Standard State.
C1H4O1<G> T.C.R.A.S. Class: 5
C1H4O1<G> CH3OH<G>
METHANOL <GAS>
C1O1<G> JANAF THERMOCHEMICAL TABLES SGTE **
C1O1<G> CO<G>
CARBON MONOXIDE <GAS>
STANDARD STATE : CODATA KEY VALUE. /CP FROM JANAF PUB. 9/65
C1O2<G> T.C.R.A.S. Class: 2
C1O2<G> CO2<G>
CARBON DIOXIDE <GAS>
C2<G> T.C.R.A.S. Class: 2
C2<G>
CARBON Diatomic Gas.
C2H1<G> T.C.R.A.S. Class: 6
C2H1<G> C2H<G>
CCH RADICAL <GAS>
C2H2<G> T.C.R.A.S. Class: 2
C2H2<G>
ACETYLENE (ETYLENE). Gaseous Standard State.
C2H2O1<G> T.C.R.A.S. Class: 6
C2H2O1<G>
OXIRENE
S298 corrected and cp refitted
due to corrected data in IVTAN2000 7/2002
C2H3<G> T.C.R.A.S. Class: 6
C2H3<G>
DICARBON TRIHYDRIDE, Gaseous Standard State.
C2H4<G> T.C.R.A.S. Class: 6
C2H4<G>
ETHYLENE. Gaseous Standard State.
C2H4O1_ACETALDEHYDE<G> T.C.R.A.S. Class: 5
C2H4O1_ACETALDEHYDE<G>
C2H4O1_OXIRANE<G> T.C.R.A.S. Class: 6
C2H4O1_OXIRANE<G>
S298 corrected and cp refitted
due to corrected data in IVTAN2000 7/2002
C2H4O2_ACETICACID<G> T.C.R.A.S. Class: 5
C2H4O2_ACETICACID<G>
C2H4O2_DIOXETANE<G> T.C.R.A.S. Class: 6
C2H4O2_DIOXETANE<G>
S298 corrected and cp refitted
due to corrected data in IVTAN2000 7/2002

```

typing error corrected 12/06  
 C2H4O3\_123TRIOXOLANE<G> T.C.R.A.S. Class: 7  
 C2H4O3\_123TRIOXOLANE<G>  
 S298 corrected and cp refitted  
 due to corrected data in IVTAN2000 7/2002  
 C2H4O3\_124TRIOXOLANE<G> T.C.R.A.S. Class: 7  
 C2H4O3\_124TRIOXOLANE<G>  
 S298 corrected and cp refitted  
 due to corrected data in IVTAN2000 7/2002  
 typing error corrected 12/06  
 C2H5<G> T.C.R.A.S. Class: 6  
 C2H5<G>  
 ETHYL radical. Gaseous Standard State.  
 C2H6<G> T.C.R.A.S. Class: 6  
 C2H6<G>  
 ETHANE. Gaseous Standard State.  
 C2H6O1<G> T.C.R.A.S. Class: 6  
 C2H6O1<G> C2H6O<G>  
 ETHANOL <GAS>  
 C2H6O2<G> THERMODATA  
 C2H6O2<G>  
 E-GLYCOL <GAS>.Data revised by THDA.  
 C2O1<G> T.C.R.A.S. Class: 5  
 C2O1<G> C2O<G>  
 C3<G> T.C.R.A.S. Class: 6  
 C3<G>  
 CARBON <TRIATOMIC GAS>  
 C3H1<G> T.C.R.A.S. Class: 6  
 C3H1<G> C3H<G>  
 2-PROPYNYLIDYNE (gaseous state)  
 S298 corrected and cp refitted  
 due to corrected data in IVTAN2000 7/2002  
 C3H4\_1<G> STULL WESTRUM SINKE 1969 SGTE  
 C3H4\_1<G>  
 ALLENE = 1,2-PROPADIENE (gaseous state)  
 EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.  
 C3H4\_2<G> STULL WESTRUM SINKE 1969 SGTE  
 C3H4\_2<G>  
 PROPYNE (METHYLACETYLENE) (gaseous state)  
 EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.  
 C3H6O1<G> THERMODATA 01/93  
 C3H6O1<G> ACETONE gas  
 ACETONE (gaseous state)  
 28/01/93  
 C3H6\_1<G> T.C.R.A.S. Class: 6 4.09.85  
 C3H6\_1<G> Cyclopropane gas  
 C3H6\_2<G> STULL WESTRUM SINKE 1969 SGTE  
 C3H6\_2<G> PROPENE gas  
 PROPENE (gaseous state)  
 EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.  
 C3H8<G> THERMODATA SGTE  
 C3H8<G> PROPANE gas  
 PROPANE <Gaseous Standard State>  
 C3O2<G> T.C.R.A.S. Class: 6  
 C3O2<G>  
 C4<G> T.C.R.A.S. Class: 7  
 C4<G>  
 C4H1<G> T.C.R.A.S. Class: 6  
 C4H1<G> C4H<G> 1,3-BUTADIYNYL gas  
 1,3-BUTADIYNYL (Gaseous Standard State).  
 Data provided by T.C.R.A.S. in 2000  
 C4H10\_1<G> T.C.R.A.S. Class: 4  
 C4H10\_1<G> BUTANE gas  
 BUTANE (Gaseous Standard State).  
 Data provided by T.C.R.A.S. in 2000  
 C4H10\_2<G> T.C.R.A.S. Class: 4  
 C4H10\_2<G> METHYLPROPANE N-BUTANE gas  
 METHYLPROPANE N-BUTANE (Gaseous Standard State).  
 Data provided by T.C.R.A.S. in 2000  
 C4H2\_1<G> THERMODATA 1978 ST  
 C4H2\_1<G> 1,3-BUTADIYNE gas  
 C4H2\_2<G> THERMODATA 06/93 ST  
 C4H2\_2<G> BUTADIYNE (BIACETYLENE) gas  
 C4H4\_1<G> T.C.R.A.S. Class: 6  
 C4H4\_1<G> 1,3-CYCLOBUTADIENE gas.  
 1,3-CYCLOBUTADIENE. Gaseous Standard State.  
 Data provided by T.C.R.A.S. in 2000  
 C4H4\_2<G> STULL WESTRUM SINKE 1969 SGTE  
 C4H4\_2<G> 1-BUTEN-3-YNE VINYLACETYLENE gas  
 1-BUTEN-3-YNE VINYLACETYLENE. Gaseous Standard State.  
 EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.  
 C4H6\_1<G> STULL WESTRUM SINKE 1969 SGTE  
 C4H6\_1<G>  
 1,2-BUTADIENE  
 EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.  
 C4H6\_2<G> STULL WESTRUM SINKE 1969 SGTE  
 C4H6\_2<G>  
 1,3-BUTADIENE  
 EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.  
 C4H6\_3<G> STULL WESTRUM SINKE 1969 SGTE  
 C4H6\_3<G>  
 1-BUTYNE ETHYLACETYLENE  
 EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.  
 C4H6\_4<G> STULL WESTRUM SINKE 1969 SGTE  
 C4H6\_4<G>  
 2-BUTYNE DIMETHYLACETYLENE  
 EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.  
 C4H6\_5<G> T.C.R.A.S. Class: 6  
 C4H6\_5<G>  
 CYCLOBUTENE. Data provided by T.C.R.A.S. in 2000  
 C4H8\_1<G> THERMODATA 04/98 TC  
 C4H8\_1<G> 1-BUTENE gas  
 C4H8\_2<G> THERMODATA 04/98 TC  
 C4H8\_2<G> (E)-2-BUTENE gas  
 C4H8\_3<G> THERMODATA 04/98 TC  
 C4H8\_3<G> (Z)-2-BUTENE gas  
 C4H8\_4<G> THERMODATA 04/98 TC  
 C4H8\_4<G> CYCLOBUTANE gas  
 C4H8\_5<G> THERMODATA 04/98 TC  
 C4H8\_5<G> 2-METHYLPROPENE gas  
 C4H8\_6<G> THERMODATA 04/98 TC  
 C4H8\_6<G> METHYLCYCLOPROPANE gas  
 C5<G> T.C.R.A.S. Class: 7  
 C5<G>  
 C60<G> MHR-95  
 C60<G>



Data processed from [94Kor/Sid] M.V. Korobov, L.N. sidorov, J. Chem. Thermo, 26, 61-73 (1994). Recalculated from the rotational data in [91McK] and vibration frequencies in [94Kor/Sid]. Note that a frequency with degeneracy 5 is missing from list in [94Kor/Sid]; taken to be 419 cm<sup>-1</sup>, 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<sup>-1</sup> for the reaction 60Cg>=C60<g> and that given by [94Kor/Sid] in their Table 5, -8950 J mol K<sup>-1</sup>. Enthalpy of formation: DfH = 2588 kJ/mol from DsubH(298.15K) = 166 +/- 11 kJ mol<sup>-1</sup> [94Kor/Sid]. Vapour pressure values reproduced very well.  
[91McK] J.T. McKinnon, J. Phys. Chem. 95 8941(1993).

C6H6<G> T.C.R.A.S. Class: 5  
C6H6<G> BENZENE gas  
BENZENE (Gaseous Standard State).  
Data provided by T.C.R.A.S. in 2000

C6H6O1<G> THERMODYNAMICS 01/93  
C6H6O1<G>  
PHENOL gas  
28/01/93

H1<G> JANAF 1982; ASSESSMENT DATED 3/77 SGTE \*\*  
H1<G> H<G>  
HYDROGEN <MONATOMIC GAS>  
H1O1<G> T.C.R.A.S. Class: 1  
H1O1<G> OH<G>  
H1O2<G> T.C.R.A.S. Class: 4  
H1O2<G> HO2<G>  
H2<G> JANAF THERMOCHEMICAL TABLES SGTE \*\*  
H2<G> H2<G>  
HYDROGEN<G>  
STANDARD STATE FROM CODATA KEY VALUES. CP FROM JANAF PUB. 3/61  
H2O1<G> T.C.R.A.S. Class: 1  
H2O1<G> H2O<G>  
WATER <GAS>, STEAM  
H2O2<G> JANAF SECOND EDIT SGTE  
H2O2<G> H2O2<G>  
HYDROGEN PEROXIDE <GAS>  
O1<G> TCRAS 02/06/80  
O1<G> O<G>  
O2<G> TCRAS 21/06/90  
O2<G>  
OXYGEN Gaseous Standard State.  
O3<G> TCRAS 02/06/80  
O3<G>  
OZONE Gaseous Standard State.  
C1H2O2<L> THERMODYNAMICS 01/93  
C1H2O2\_Liquid HCOOH\_Liquid  
FORMIC ACID MONOMERIC  
28/01/93  
C1H4O1<L> I. BARIN 3rd. Edition  
C1H4O1\_Liquid CH3OH\_Liquid  
METHANOL (Liquid). H298 and S298 modified.  
C2H4O2<L> THERMODYNAMICS 01/93  
C2H4O2\_Liquid  
ACETIC ACID (Liquid)  
28/01/93 Tb=389K.  
C2H6O1<L> THERMODYNAMICS 01/93  
C2H6O1\_Liquid C2H6O\_Liquid  
ETHANOL (Liquid)  
28/01/93  
C2H6O2<L> THERMODYNAMICS  
C2H6O2\_Liquid  
E-GLYCOL (Liquid)  
Data revised by THDA.  
C60 MHR-95  
C60  
Data processed from [94Kor/Sid] M.V. Korobov, L.N. sidorov, J. Chem. The  
Fitted to the data in [94Kor/Sid], who took the phase transition at 257K  
that [94Kor/Sid] do not give an explicit value for S(298.15K).  
S(298.15K) = 422.6 J mol K<sup>-1</sup> 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<sup>-1</sup>.  
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> THERMODYNAMICS 04/99 BC  
C6H6\_Liquid BENZENE Liquid  
C1<DIAMOND> S.G.T.E. \*\*  
C\_DIAMOND  
<DIAMOND>  
Data from SGTE Unary DB, data added by atd 7/9/95, H298-H0 taken  
from 1994 database (ex THERMODYNAMICS 01/93)  
C1<GRAPHITE> S.G.T.E. \*\*  
C\_GRAPHITE  
Data from SGTE Unary DB, pressure dependent data added by atd 7/9/95  
H2O1<L> T.C.R.A.S. Class: 4  
H2O1\_Liquid H2O\_Liquid Pure\_Water  
WATER  
T.C.R.A.S. Class: 4 cp modified by atd 12/9/94 and 5/7/2002  
H2O2<L> THERMODYNAMICS 01/93  
H2O2\_Liquid H2O2\_Liquid  
HYDROGEN PEROXIDE  
28/01/93

-OK-

**TDB\_SSUB5:** go p-3  
... the command in full is GOTO\_MODULE

POLY version 3.32  
**POLY\_3:** l-st  
... the command in full is LIST\_STATUS

**Option /CPS/:**  
\*\*\* STATUS FOR ALL COMPONENTS

COMPONENT	STATUS	REF. STATE	T(K)	P(Pa)
VA	ENTERED	SER		
C	ENTERED	SER		
H	ENTERED	SER		
O	ENTERED	SER		

\*\*\* STATUS FOR ALL PHASES

PHASE	STATUS	DRIVING FORCE	MOLES
H2O2_L	ENTERED	0.000000E+00	0.000000E+00
H2O1_L	ENTERED	0.000000E+00	0.000000E+00
GRAPHITE_L	ENTERED	0.000000E+00	0.000000E+00

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GRAPHITE          ENTERED      0.000000E+00    0.000000E+00
DIAMOND           ENTERED      0.000000E+00    0.000000E+00
C6H6_L           ENTERED      0.000000E+00    0.000000E+00
C60_S            ENTERED      0.000000E+00    0.000000E+00
C2H6O2_L         ENTERED      0.000000E+00    0.000000E+00
C2H6O1_L         ENTERED      0.000000E+00    0.000000E+00
C2H4O2_L         ENTERED      0.000000E+00    0.000000E+00
C1H4O1_L         ENTERED      0.000000E+00    0.000000E+00
C1H2O2_L         ENTERED      0.000000E+00    0.000000E+00
GAS               ENTERED      0.000000E+00    0.000000E+00
*** STATUS FOR ALL SPECIES
C                 ENTERED      C3H6O1          ENTERED
C1H1             ENTERED      C3H6_1          ENTERED
C1H1O1           ENTERED      C3H6_2          ENTERED
C1H1O2           ENTERED      C3H8            ENTERED
C1H2             ENTERED      C3O2            ENTERED
C1H2O1           ENTERED      C4              ENTERED
C1H2O2           ENTERED      C4H1            ENTERED
C1H2O2_CIS       ENTERED      C4H10_1         ENTERED
C1H2O2_DIOXIRANE ENTERED      C4H10_2         ENTERED
C1H2O2_TRANS     ENTERED      C4H2_1          ENTERED
C1H3             ENTERED      C4H2_2          ENTERED
C1H3O1_CH2OH     ENTERED      C4H4_1          ENTERED
C1H3O1_CH3O      ENTERED      C4H4_2          ENTERED
C1H4             ENTERED      C4H6_1          ENTERED
C1H4O1           ENTERED      C4H6_2          ENTERED
C1O1             ENTERED      C4H6_3          ENTERED
C1O2             ENTERED      C4H6_4          ENTERED
C2              ENTERED      C4H6_5          ENTERED
C2H1             ENTERED      C4H8_1          ENTERED
C2H2             ENTERED      C4H8_2          ENTERED
C2H2O1           ENTERED      C4H8_3          ENTERED
C2H3             ENTERED      C4H8_4          ENTERED
C2H4             ENTERED      C4H8_5          ENTERED
C2H4O1_ACETALDEHYDE ENTERED      C4H8_6          ENTERED
C2H4O1_OXIRANE   ENTERED      C5              ENTERED
C2H4O2           ENTERED      C6O             ENTERED
C2H4O2_ACETICACID ENTERED      C6H6            ENTERED
C2H4O2_DIOXETANE ENTERED      C6H6O1          ENTERED
C2H4O3_123TRIOXOLANE ENTERED      H              ENTERED
C2H4O3_124TRIOXOLANE ENTERED      H1O1           ENTERED
C2H5             ENTERED      H1O2           ENTERED
C2H6             ENTERED      H2              ENTERED
C2H6O1           ENTERED      H2O1           ENTERED
C2H6O2           ENTERED      H2O2           ENTERED
C2O1             ENTERED      O              ENTERED
C3              ENTERED      O2             ENTERED
C3H1            ENTERED      O3             ENTERED
C3H4_1          ENTERED      VA             ENTERED
C3H4_2          ENTERED
POLY_3: @@ We need to know the heat content of C3H8<G> at room temperature.
POLY_3: @@ This is a simple number to look up in a table but actually quite
POLY_3: @@ tricky to calculate as pure C3H8 at room temperature does not
POLY_3: @@ represent an equilibrium state. However, one can obtain it by
POLY_3: @@ the following procedure.
POLY_3: s-c t=298.15,p=1e5,n(o)=1e-10
... the command in full is SET_CONDITION
POLY_3: s-i-a n(c3h8)=1
... the command in full is SET_INPUT_AMOUNTS
POLY_3: c-s p *=sus
... the command in full is CHANGE_STATUS
POLY_3: c-s p gas
... the command in full is CHANGE_STATUS
Status: /ENTERED/:
Start value, number of moles /0/:
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      74 grid points in      0 s
Found the set of lowest grid points in      0 s
Calculated POLY solution      0 s, total time      0 s
POLY_3: @@ The equilibrium state at room temperature is listed
POLY_3: l-e,,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium =      1, label A0 , database: SSUB5

Conditions:
T=298.15, P=1E5, N(O)=1E-10, N(C)=3, N(H)=8
DEGREES OF FREEDOM 0

Temperature      298.15 K (      25.00 C), Pressure 1.000000E+05
Number of moles of components 1.10000E+01, Mass in grams 4.40962E+01
Total Gibbs energy -2.20108E+05, Enthalpy -1.06064E+05, Volume 4.99502E-02

Component      Moles      W-Fraction Activity Potential Ref.stat
C               3.0000E+00  8.1715E-01 1.1356E+07 4.0271E+04 SER
H               8.0000E+00  1.8285E-01 3.4211E-08 -4.2615E+04 SER
O               1.0000E-10  3.6282E-11 1.2651E-49 -2.7911E+05 SER

GAS              Status ENTERED      Driving force 0.0000E+00
Moles 1.1000E+01, Mass 4.4096E+01, Volume fraction 1.0000E+00 Mass fractions:
C 8.17145E-01 H 1.82855E-01 O 3.62820E-11
Constitution:
C1H4            9.90348E-01 C2H6O1      1.83029E-24 C4H6_3      1.00000E-30
C6O             8.16678E-03 C1H4O1      1.08754E-24 C2H4O1_OXIRA 1.00000E-30
C6H6            1.38456E-03 C1H2O1      4.96084E-27 C4H6_5      1.00000E-30
C2H6            1.00313E-04 C1H2O2_CIS  4.88436E-27 C5          1.00000E-30
C3H8            5.44582E-07 C4H6_4      3.94602E-28 C2H3        1.00000E-30
C4H10_2         3.84975E-08 C3H4_2      6.04110E-29 C2H2O1      1.00000E-30
H2              7.83769E-09 C2H5        1.32230E-29 C2H2        1.00000E-30
C4H10_1         6.16323E-09 C1H2O2_TRANS 6.61825E-30 C2H1        1.00000E-30
C1O2            2.32090E-11 C3H4_1      2.45341E-30 C2          1.00000E-30
H2O1            2.50979E-12 C4H6_1      2.07866E-30 H           1.00000E-30
C1O1            7.01016E-13 C           1.00000E-30 H1O1        1.00000E-30
C4H8_5          6.29486E-14 C3O2        1.00000E-30 H1O2        1.00000E-30
C3H6_2         5.52670E-14 C4          1.00000E-30 H2O2        1.00000E-30
C2H4            3.33175E-14 C4H1        1.00000E-30 C1H3O1_CH3O 1.00000E-30
C4H8_2         7.83367E-15 C4H2_1      1.00000E-30 C1H3O1_CH2OH 1.00000E-30
C4H8_3         3.33692E-15 C3H1        1.00000E-30 C1H3        1.00000E-30
C4H8_1         4.53470E-16 C3          1.00000E-30 O           1.00000E-30
C6H6O1         1.02341E-18 C2O1        1.00000E-30 C1H2O2_DIOXI 1.00000E-30
C3H6O1         9.99430E-20 C2H6O2      1.00000E-30 O2          1.00000E-30
C3H6_1         2.70389E-21 C4H2_2      1.00000E-30 O3          1.00000E-30
C4H8_6         1.07592E-21 C4H4_1      1.00000E-30 C1H2        1.00000E-30
C4H6_2         4.91032E-22 C4H4_2      1.00000E-30 C1H1O2      1.00000E-30

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C2H4O1_ACETA 1.25014E-22  C2H4O3_124TR 1.00000E-30  C1H1O1      1.00000E-30
C4H8_4        2.10624E-23  C2H4O3_123TR 1.00000E-30  C1H1      1.00000E-30
C2H4O2_ACETI 9.64309E-24  C2H4O2_DIOXE 1.00000E-30
POLY_3: @@ The enthalpy for the system is
POLY_3: sh h
... the command in full is SHOW_VALUE
H=-106064.27
POLY_3:Hit RETURN to continue
POLY_3: @@ But we want a gas with just C3H8. Use the set-all-startvalues command.
POLY_3: s-a-s
... the command in full is SET_ALL_START_VALUES
Automatic start values for phase constituents? /N/: n

Should GAS be stable? /Y/: 1
Major constituent(s): C3H8
POLY_3: sh h
... the command in full is SHOW_VALUE
H=-99369.211
POLY_3: @@ The difference in H for the two calculations is actually not very large.
POLY_3: @@ The value is approximate but rather good as the enthalpy is calculated
POLY_3: @@ for the following gas constitution
POLY_3: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: SSUB5

Conditions:
T=298.15, P=1E5, N(O)=1E-10, N(C)=3, N(H)=8
DEGREES OF FREEDOM 0

Temperature 298.15 K ( 25.00 C), Pressure 1.000000E+05
Number of moles of components 1.07452E+01, Mass in grams 4.32989E+01
Total Gibbs energy -1.78514E+05, Enthalpy -9.93692E+04, Volume 2.43004E-02

Component      Moles      W-Fraction  Activity   Potential  Ref.stat
C                2.9419E+00  8.1606E-01  1.1356E+07  4.0271E+04  SER
H                7.7967E+00  1.8149E-01  3.4211E-08  -4.2615E+04  SER
O                6.6216E-03  2.4467E-03  1.2651E-49  -2.7911E+05  SER

GAS              Status ENTERED   Driving force  0.0000E+00
Moles 1.0745E+01, Mass 4.3299E+01, Volume fraction 1.0000E+00  Mass fractions:
C 8.16064E-01 H 1.81489E-01 O 2.44670E-03
Constitution:
C3H8      9.70396E-01  C4H4_2      1.35135E-04  C2H4O2_ACETI 1.35135E-04
C          1.35135E-04  C4H4_1      1.35135E-04  C2H4O1_OXIRA 1.35135E-04
O2         1.35135E-04  C4H2_2      1.35135E-04  C2H4O1_ACETA 1.35135E-04
O          1.35135E-04  C4H2_1      1.35135E-04  C2H4         1.35135E-04
H2O2       1.35135E-04  C4H10_2     1.35135E-04  C2H3         1.35135E-04
H2O1       1.35135E-04  C4H10_1     1.35135E-04  C2H2O1       1.35135E-04
H2         1.35135E-04  C4H1_       1.35135E-04  C2H2         1.35135E-04
H1O2       1.35135E-04  C4          1.35135E-04  C2H1         1.35135E-04
H1O1       1.35135E-04  C3O2        1.35135E-04  C2           1.35135E-04
H          1.35135E-04  O3          1.35135E-04  C1O2         1.35135E-04
C6H6O1     1.35135E-04  C3H6_2      1.35135E-04  C1O1         1.35135E-04
C6H6       1.35135E-04  C3H6_1      1.35135E-04  C1H4O1       1.35135E-04
C6O        1.35135E-04  C3H6O1      1.35135E-04  C1H4         1.35135E-04
C5         1.35135E-04  C3H4_2      1.35135E-04  C1H3O1_CH3O 1.35135E-04
C4H8_6     1.35135E-04  C3H4_1      1.35135E-04  C1H3O1_CH2OH 1.35135E-04
C4H8_5     1.35135E-04  C3H1_       1.35135E-04  C1H3         1.35135E-04
C4H8_4     1.35135E-04  C3          1.35135E-04  C1H2O2_TRANS 1.35135E-04
C4H8_3     1.35135E-04  C2O1        1.35135E-04  C1H2O2_DIOXI 1.35135E-04
C4H8_2     1.35135E-04  C2H6O2      1.35135E-04  C1H2O2_CIS   1.35135E-04
C4H8_1     1.35135E-04  C2H6O1      1.35135E-04  C1H2O1       1.35135E-04
C4H6_5     1.35135E-04  C2H6        1.35135E-04  C1H2         1.35135E-04
C4H6_4     1.35135E-04  C2H5        1.35135E-04  C1H1O2       1.35135E-04
C4H6_3     1.35135E-04  C2H4O3_124TR 1.35135E-04  C1H1O1       1.35135E-04
C4H6_2     1.35135E-04  C2H4O3_123TR 1.35135E-04  C1H1         1.35135E-04
C4H6_1     1.35135E-04  C2H4O2_DIOXE 1.35135E-04
POLY_3:Hit RETURN to continue
POLY_3: @@ We now have the initial amount of heat. Assuming an excess
POLY_3: @@ of oxygen we can calculate the temperature where the
POLY_3: @@ heat content would be the same
POLY_3: sh h
... the command in full is SHOW_VALUE
H=-99369.211
POLY_3: @@ H is just 11 times HM as there are 11 atoms in C3H8, save that value
POLY_3: @@ in a variable
POLY_3: enter var h298=h;
... the command in full is ENTER_SYMBOL
POLY_3: sh h298
... the command in full is SHOW_VALUE
H298=-99369.211
POLY_3: @@ If all carbon and hydrogen react with oxygen we need 7 oxygen atoms
POLY_3: @@ to form 3 moles C1O and 4 moles of H2O, add some oxygen in excess
POLY_3: s-c n(o)=9
... the command in full is SET_CONDITION
POLY_3: @@ Set the heat content as condition and remove the condition on t
POLY_3: s-c h=h298
... the command in full is SET_CONDITION
POLY_3: s-c t
... the command in full is SET_CONDITION
Value /298.15/: none
POLY_3: l-c
... the command in full is LIST_CONDITIONS
P=1E5, N(O)=9, N(C)=3, N(H)=8, H=H298
DEGREES OF FREEDOM 0
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 74 grid points in 0 s
152 ITS, CPU TIME USED 0 SECONDS
POLY_3: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: SSUB5

Conditions:
P=1E5, N(O)=9, N(C)=3, N(H)=8, H=H298
DEGREES OF FREEDOM 0

Temperature 3104.37 K ( 2831.22 C), Pressure 1.000000E+05
Number of moles of components 2.00000E+01, Mass in grams 1.88087E+02
Total Gibbs energy -7.70908E+06, Enthalpy -9.93692E+04, Volume 2.20523E+00

Component      Moles      W-Fraction  Activity   Potential  Ref.stat

```

```
C          3.0000E+00  1.9158E-01  9.3493E-09 -4.7720E+05 SER
H          8.0000E+00  4.2869E-02  7.7490E-06 -3.0375E+05 SER
O          9.0000E+00  7.6555E-01  6.4120E-08 -4.2750E+05 SER
```

```
GAS          Status ENTERED      Driving force  0.0000E+00
Moles 2.0000E+01, Mass 1.8809E+02, Volume fraction 1.0000E+00  Mass fractions:
O  7.65554E-01  C  1.91576E-01  H  4.28695E-02
```

```
Constitution:
H2O1      3.17884E-01  C2H2      1.13693E-15  C3H6O1      1.00000E-30
ClO1      2.27661E-01  ClH2O2_DIOXI  7.93238E-16  C3H6_1      1.00000E-30
ClO2      1.23475E-01  C2H1      8.87885E-17  C3H6_2      1.00000E-30
H1O1      8.79356E-02  C3O2      8.69739E-17  C3H8        1.00000E-30
H2        7.64745E-02  C2        1.58189E-17  C4          1.00000E-30
O2        6.60347E-02  C2H2O1    2.51164E-18  C4H1        1.00000E-30
H          5.96672E-02  C2H3      2.70073E-19  C4H10_1     1.00000E-30
O          4.08218E-02  C2H4O1_ACETA 1.21158E-20  C4H10_2     1.00000E-30
H1O2      4.27603E-05  C2H4      1.11202E-20  C4H4_1      1.00000E-30
H2O2      1.61649E-06  C2H4O2_ACETI 7.57727E-21  C4H8_4      1.00000E-30
ClH1O1     9.35206E-07  C3H1      9.63256E-23  C4H8_5      1.00000E-30
ClH1O2     6.81909E-07  C3        6.39018E-23  C4H4_2      1.00000E-30
O3         3.02268E-08  C2H4O1_OXIRA 1.09569E-23  C4H6_1      1.00000E-30
ClH2O2_CIS  1.60411E-08  C2H5      2.13496E-24  C4H6_2      1.00000E-30
ClH2O2_TRANS 8.96990E-09  C2H6      2.28920E-26  C4H6_3      1.00000E-30
ClH2O1     7.23694E-09  C2H6O1    6.22800E-27  C4H6_4      1.00000E-30
C          5.44356E-11  C2H6O2    8.36793E-28  C4H8_6      1.00000E-30
ClH1       5.72382E-12  C3H4_2    5.27771E-28  C4H6_5      1.00000E-30
ClH2       2.82162E-12  C3H4_1    2.83571E-28  C5          1.00000E-30
ClH3       2.07810E-12  C2H4O2_DIOXE 1.26547E-29  C6O         1.00000E-30
C2O1       1.16914E-12  C2H4O3_124TR 2.44217E-30  C4H8_1      1.00000E-30
ClH3O1_CH2OH 8.91882E-13  C4H2_1    2.35081E-30  C6H6        1.00000E-30
ClH4       1.78630E-13  C4H2_2    2.34436E-30  C6H6O1      1.00000E-30
ClH3O1_CH3O 1.92065E-14  C4H8_3    1.00000E-30  C4H8_2      1.00000E-30
ClH4O1     9.71550E-15  C2H4O3_123TR 1.00000E-30
```

```
POLY_3: @@ The adiabatic temperature is
POLY_3: sh t
... the command in full is SHOW_VALUE
T=3104.3748
POLY_3:Hit RETURN to continue
POLY_3: @@ Now calculate how the adiabatic temperature varies with
POLY_3: @@ the amount of oxygen
POLY_3: s-a-v 1 n(o) 5 10
... the command in full is SET_AXIS_VARIABLE
Increment /.125/:
POLY_3: save tcex22 y
... the command in full is SAVE_WORKSPACES
POLY_3: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 9.00000
...OK

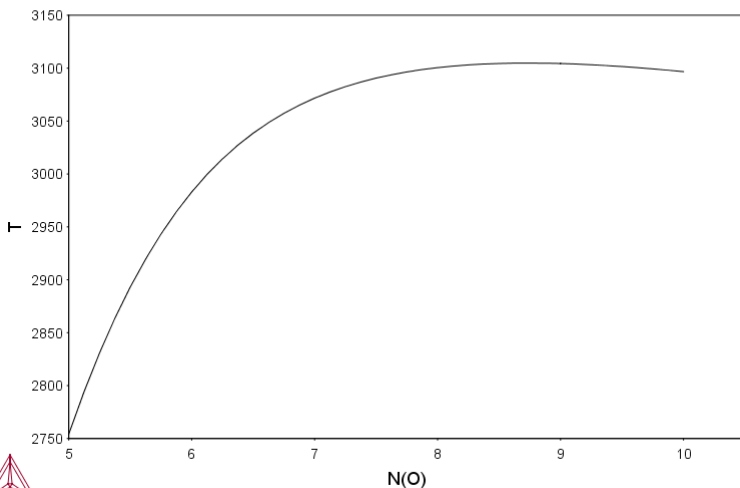
Phase Region from 9.00000 for:
GAS
Global test at 1.00000E+01 .... OK
Terminating at 10.00000
Calculated 11 equilibria

Phase Region from 9.00000 for:
GAS
Global test at 8.00000E+00 .... OK
Global test at 6.75000E+00 .... OK
Global test at 5.50000E+00 .... OK
Terminating at 5.00000
Calculated 35 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex22\tcex
22.POLY3
POLY_3: post
```

POLY-3 POSTPROCESSOR VERSION 3.2

```
POST:
POST: s-d-a x n(o)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 22a
POST: plot
... the command in full is PLOT DIAGRAM
example 22a
```

2016.05.16.13.48.41  
SSUBS: C, H, O  
P=1E5, N(C)=3, N(H)=8, H=H298



```
POST:
POST:Hit RETURN to continue
POST: @@ Plot how the gas constitution changes
```

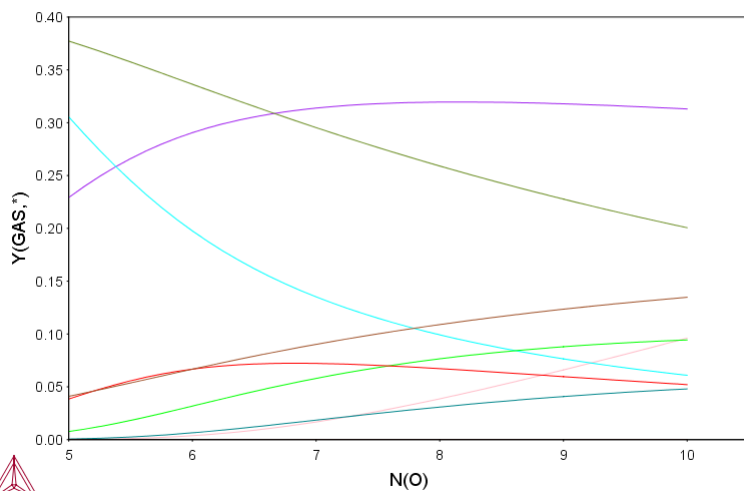
```

POST: s-d-a y y(gas,*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: set-title example 22b
POST:
POST: plot
... the command in full is PLOT DIAGRAM

```

example 22b

2016.05.16.13.48.41  
SSUB5: C, H, O  
P=1E5, N(C)=3, N(H)=8, H=H298



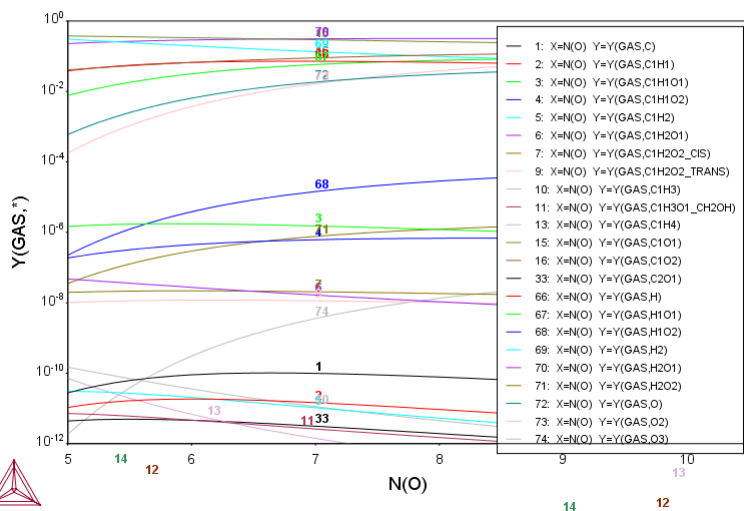
```

POST:
POST:Hit RETURN to continue
POST: @@ Add labels and logarithmic fraction scale
POST: s-lab d
... the command in full is SET_LABEL_CURVE_OPTION
POST: s-a-ty y log
... the command in full is SET_AXIS_TYPE
POST: s-s y n 1e-12 1
... the command in full is SET_SCALING_STATUS
POST: set-title example 22c
POST:
POST: plot
... the command in full is PLOT DIAGRAM

```

example 22c

2016.05.16.13.48.42  
SSUB5: C, H, O  
P=1E5, N(C)=3, N(H)=8, H=H298



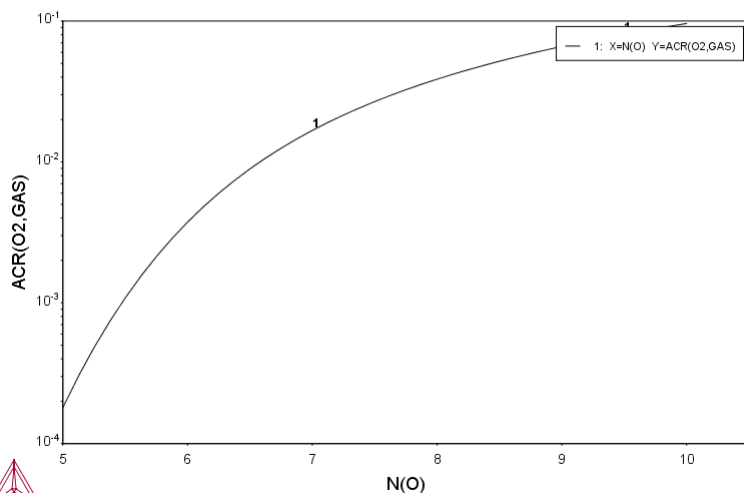
```

POST:
POST:Hit RETURN to continue
POST: @@ Plot how the oxygen partial pressure changes
POST: s-d-a y acr(o2,gas)
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 22d
POST:
POST: plot
... the command in full is PLOT DIAGRAM

```

# example 22d

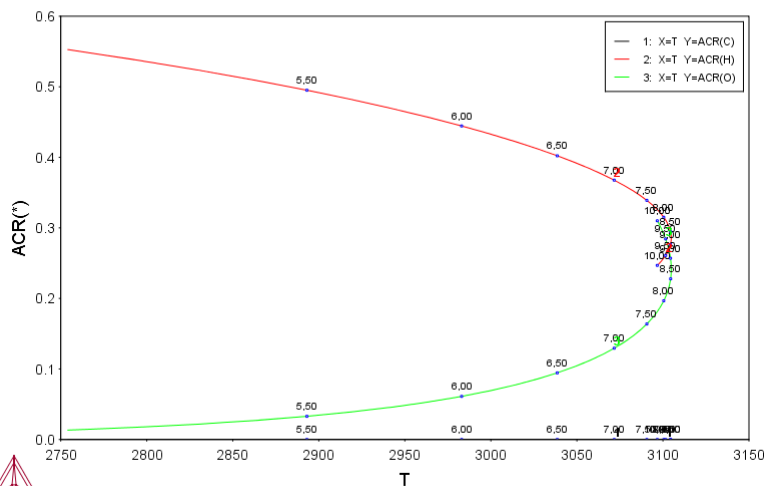
2016.05.16.13.48.42  
SSUB5: C, H, O  
P=1E5, N(C)=3., N(H)=8., H=H298



```
POST:
POST:Hit RETURN to continue
POST: @@ Plot how the activities of the components change with temperature
POST: @@ Note that the oxygen content changes also ...
POST: @@ We must set reference states
POST: set-ref-state o gas * 1e5
... the command in full is SET_REFERENCE_STATE
You should set-diagram-axis for the activity/potential after this!
POST: set-ref-state h gas * 1e5
... the command in full is SET_REFERENCE_STATE
You should set-diagram-axis for the activity/potential after this!
POST: set-ref-state c c_s * 1e5
... the command in full is SET_REFERENCE_STATE
You should set-diagram-axis for the activity/potential after this!
POST: s-d-a x t
... the command in full is SET_DIAGRAM_AXIS
POST: s-a-ty y lin
... the command in full is SET_AXIS_TYPE
POST: s-d-a z n(o)
... the command in full is SET_DIAGRAM_AXIS
POST: s-s z n 5 10
... the command in full is SET_SCALING_STATUS
POST: s-d-a y acr(*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: set-title example 22e
POST:
POST: plot
... the command in full is PLOT DIAGRAM
```

# example 22e

2016.05.16.13.48.43  
SSUB5: C, H, O  
P=1E5, N(C)=3., N(H)=8., H=H298



```
POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex23

```
AboutMACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex23\tcex23.TCM" set-echo
SYS: @@
SYS: @@
SYS: @@ Calculation of T-zero and paraequilibria in a low alloyed steel
SYS: @@
SYS: set-log ex23,,,
SYS: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3: @@ Define the material
POLY_3: def-mat
... the command in full is DEFINE_MATERIAL
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
L12_FCC B2_BCC B2_VACANCY
HIGH_SIGMA DICTRA_FCC_A1 REJECTED
Database /TCFE8/: tcfe7
Current database: Steels/Fe-Alloys v7.0

VA DEFINED
L12_FCC B2_BCC B2_VACANCY
HIGH_SIGMA DICTRA_FCC_A1 REJECTED
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/: Y
1st alloying element: mn 1.5
2nd alloying element: si .3
Next alloying element: c .3
Next alloying element:
Temperature (C) /1000/: 700
VA DEFINED
L12_FCC B2_BCC B2_VACANCY
HIGH_SIGMA DICTRA_FCC_A1 REJECTED
REINITIATING GES5 .....
... the command in full is DEFINE_ELEMENTS
FE DEFINED
... the command in full is DEFINE_ELEMENTS
MN DEFINED
... the command in full is DEFINE_ELEMENTS
SI DEFINED
... the command in full is DEFINE_ELEMENTS
C DEFINED

This database has following phases for the defined system

GAS:G LIQUID:L BCC_A2
FCC_A1 HCP_A3 DIAMOND_FCC_A4
GRAPHITE CEMENTITE M23C6
M7C3 M5C2 KSI_CARBIIDE
A1_KAPPA KAPPA FE4N_LP1
FECN_CHI LAVES_PHASE_C14 M3SI
G_PHASE CR3SI FE2SI
MSI M5SI3 AL4C3
FE8SI2C SIC

Reject phase(s) /NONE/: NONE
Restore phase(s): /NONE/: NONE

.....

The following phases are retained in this system:

GAS:G LIQUID:L BCC_A2
FCC_A1 HCP_A3 DIAMOND_FCC_A4
GRAPHITE CEMENTITE M23C6
M7C3 M5C2 KSI_CARBIIDE
A1_KAPPA KAPPA FE4N_LP1
FECN_CHI LAVES_PHASE_C14 M3SI
G_PHASE CR3SI FE2SI
MSI M5SI3 AL4C3
FE8SI2C SIC

.....

OK? /Y/: Y
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

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'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
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'J. Grobner, H.L. Lukas and F. Aldinger, Calphad, 20 (1996), 247-254; Si-C
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'W. Huang, Calphad, 13 (1989), 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
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Fe-Si and Fe-Si-C'
'J. Miettinen and B. Hallstedt, Calphad, 22 (1998), 231-256; Fe-Si and Fe
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hard mater, Vol. 12, pp. 121-127; Molar volumes'
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Molar volumes'
'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
```

```

'W. Huang, Metall. Trans. A, 21A (1990), 2115-2123; TRITA-MAC 411 (Rev
1989); C-FE-MN'
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'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Cementite'
'P. Villars and L.D. Calvert (1985). Pearsons handbook of crystallographic
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'J-O. Andersson, Metall. Trans. A, 19A (1988), 627-636 TRITA 0207 (1986);
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'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'
'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; SIGMA and M7C3'
'Thermo-Calc Software (2008): Volume data updated for TCFe6 database (TCFe
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```

'J-O. Andersson, Calphad, 12 (1988), 9-23; TRITA 0321 (1986); C-FE-MO'

'D. Connetable, J. Lacaze, P. Maugis and B. Sundman; Calphad, Vol. 32 (2008), pp. 361-370; Al-C-Fe'

'H. Du and M. Hillert, TRITA-MAC 435 (1990); C-Fe-N'

'Estimated parameter for solubility of C in Fe4N, 1999'

'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equil., 19 (1998), 441-448; Fe-Ti'

'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; LAVES\_PHASE\_C14'

'N. Saunders, COST 507 Report (1998); Mn-Ti'

'B.-J. Lee, KRISS, unpublished research, during 1993-1995'

'I. Ansara, unpublished work (1991); Cr-Si'

'A. Markstrom, Thermo-Calc software AB, 2011'

-OK-

**Should any phase have a miscibility gap check? /N/:** N

Using global minimization procedure

Calculated	16035 grid points in	0 s
Found the set of lowest grid points in		0 s
Calculated POLY solution	0 s, total time	0 s

**POLY\_3:** l-e

... the command in full is LIST\_EQUILIBRIUM

**OUTPUT TO SCREEN OR FILE /SCREEN/:**

**Options /VWCS/:**

Output from POLY-3, equilibrium = 1, label A0 , database: TCFe7

Conditions:

T=973.15, W(MN)=1.5E-2, W(SI)=3E-3, W(C)=3E-3, P=1E5, N=1

DEGREES OF FREEDOM 0

Temperature 973.15 K ( 700.00 C), Pressure 1.000000E+05

Number of moles of components 1.00000E+00, Mass in grams 5.50671E+01

Total Gibbs energy -4.16088E+04, Enthalpy 2.38836E+04, Volume 7.24185E-06

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
C	1.3754E-02	3.0000E-03	2.2665E-01	-1.2010E+04	SER
FE	9.6533E-01	9.7900E-01	6.6031E-03	-4.0620E+04	SER
MN	1.5035E-02	1.5000E-02	6.5723E-05	-7.7919E+04	SER
SI	5.8820E-03	3.0000E-03	2.1018E-10	-1.8030E+05	SER

BCC\_A2 Status ENTERED Driving force 0.0000E+00

Moles 7.4142E-01, Mass 4.1252E+01, Volume fraction 7.4788E-01 Mass fractions:

FE 9.87818E-01 MN 8.85142E-03 SI 3.22070E-03 C 1.10187E-04

FCC\_A1 Status ENTERED Driving force 0.0000E+00

Moles 2.5248E-01, Mass 1.3742E+01, Volume fraction 2.4758E-01 Mass fractions:

FE 9.57752E-01 MN 3.35378E-02 C 6.35700E-03 SI 2.35347E-03

GRAPHITE Status ENTERED Driving force 0.0000E+00

Moles 6.1027E-03, Mass 7.3300E-02, Volume fraction 4.5452E-03 Mass fractions:

C 1.00000E+00 SI 0.00000E+00 MN 0.00000E+00 FE 0.00000E+00

**POLY\_3:** @@ Suspend some phases that normally never appear

**POLY\_3:** ch-st p gra m5c2=sus

... the command in full is CHANGE\_STATUS

**POLY\_3:**Hit RETURN to continue

**POLY\_3:** @@ Set axis for T-w(c) phase diagram

**POLY\_3:** s-a-v 1 w(c)

... the command in full is SET\_AXIS\_VARIABLE

**Min value /0/:** 0

**Max value /1/:** .01

**Increment /2.5E-04/:** 2.5E-04

**POLY\_3:** s-a-v 2 t

... the command in full is SET\_AXIS\_VARIABLE

**Min value /0/:** 800

**Max value /1/:** 1200

**Increment /10/:** 30

**POLY\_3:** save tcex23a y

.. the command in full is SAVE\_WORKSPACES

**POLY\_3:** map

Version S mapping is selected

Generating start equilibrium 1

Generating start equilibrium 2

Generating start equilibrium 3

Generating start equilibrium 4

Generating start equilibrium 5

Generating start equilibrium 6

Generating start equilibrium 7

Generating start equilibrium 8

Generating start equilibrium 9

Generating start equilibrium 10

Generating start equilibrium 11

Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Tie-lines not in the plane of calculation

Generating start point 1

Generating start point 2

Generating start point 3

Generating start point 4

Generating start point 5

Generating start point 6

Generating start point 7

Generating start point 8

Generating start point 9

Generating start point 10

Working hard

Generating start point 11

Generating start point 12

Generating start point 13

Generating start point 14



Generating start point 15  
 Generating start point 16  
 Generating start point 17  
 Generating start point 18  
 Generating start point 19  
 Generating start point 20  
 Working hard  
 Generating start point 21  
 Generating start point 22  
 Generating start point 23  
 Generating start point 24

Phase region boundary 1 at: 2.500E-04 9.455E+02  
 BCC\_A2  
 CEMENTITE  
 \*\* FCC\_A1  
 Calculated. 3 equilibria

Phase region boundary 2 at: 6.694E-05 9.437E+02  
 BCC\_A2  
 \*\* CEMENTITE  
 \*\* FCC\_A1

Phase region boundary 3 at: 6.694E-05 9.437E+02  
 BCC\_A2  
 \*\* FCC\_A1  
 Calculated 18 equilibria

Phase region boundary 4 at: 6.694E-05 9.437E+02  
 BCC\_A2  
 \*\* CEMENTITE  
 Calculated.. 10 equilibria  
 Terminating at axis limit.

Phase region boundary 5 at: 6.694E-05 9.437E+02  
 BCC\_A2  
 \*\* CEMENTITE  
 FCC\_A1  
 Calculated. 31 equilibria

Phase region boundary 6 at: 7.080E-03 9.917E+02  
 \*\* BCC\_A2  
 \*\* CEMENTITE  
 FCC\_A1

Phase region boundary 7 at: 7.080E-03 9.917E+02  
 \*\* CEMENTITE  
 FCC\_A1  
 Calculated.. 17 equilibria  
 Terminating at axis limit.

Phase region boundary 8 at: 7.080E-03 9.917E+02  
 \*\* BCC\_A2  
 FCC\_A1  
 Calculated 43 equilibria

Phase region boundary 9 at: 7.080E-03 9.917E+02  
 \*\* BCC\_A2  
 CEMENTITE  
 FCC\_A1  
 Calculated.. 13 equilibria  
 Terminating at axis limit.

Phase region boundary 10 at: 6.694E-05 9.437E+02  
 BCC\_A2  
 CEMENTITE  
 \*\* FCC\_A1  
 Calculated.. 42 equilibria  
 Terminating at axis limit.

Phase region boundary 11 at: 2.500E-04 9.455E+02  
 BCC\_A2  
 CEMENTITE  
 \*\* FCC\_A1  
 Calculated.. 41 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 12 at: 3.417E-03 9.650E+02  
 BCC\_A2  
 CEMENTITE  
 \*\* FCC\_A1  
 Calculated. 15 equilibria  
 Terminating at known equilibrium

Phase region boundary 13 at: 3.417E-03 9.650E+02  
 BCC\_A2  
 CEMENTITE  
 \*\* FCC\_A1  
 Calculated.. 28 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 14 at: 6.583E-03 9.745E+02  
 BCC\_A2  
 CEMENTITE  
 \*\* FCC\_A1  
 Calculated. 28 equilibria  
 Terminating at known equilibrium

Phase region boundary 15 at: 6.583E-03 9.745E+02  
 BCC\_A2  
 CEMENTITE  
 \*\* FCC\_A1  
 Calculated.. 16 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 16 at: 6.157E-06 8.100E+02  
 BCC\_A2  
 \*\* CEMENTITE  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 17 at: 6.157E-06 8.100E+02

```

    BCC_A2
** CEMENTITE
Calculated.          9 equilibria
Terminating at known equilibrium

Phase region boundary 18 at:  9.750E-03  9.804E+02
    BCC_A2
    CEMENTITE
** FCC_A1
Calculated.          40 equilibria
Terminating at known equilibrium

Phase region boundary 19 at:  9.750E-03  9.804E+02
    BCC_A2
    CEMENTITE
** FCC_A1
Calculated..          3 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 20 at:  6.040E-05  9.367E+02
    BCC_A2
    CEMENTITE
Calculated..          10 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 21 at:  6.040E-05  9.367E+02
    BCC_A2
    CEMENTITE
Calculated.           2 equilibria
Terminating at known equilibrium

Phase region boundary 22 at:  2.642E-03  1.063E+03
** BCC_A2
    FCC_A1
Calculated.           19 equilibria
Terminating at known equilibrium

Phase region boundary 23 at:  2.642E-03  1.063E+03
** BCC_A2
    FCC_A1
Calculated            23 equilibria

Phase region boundary 24 at:  8.904E-03  1.063E+03
** CEMENTITE
    FCC_A1
Calculated.           11 equilibria
Terminating at known equilibrium

Phase region boundary 25 at:  8.904E-03  1.063E+03
** CEMENTITE
    FCC_A1
Calculated..           7 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 26 at:  2.500E-04  1.127E+03
** BCC_A2
    FCC_A1
Calculated            22 equilibria

Phase region boundary 27 at:  2.500E-04  1.127E+03
** BCC_A2
    FCC_A1
Calculated.           29 equilibria
Terminating at known equilibrium

Phase region boundary 28 at:  3.417E-03  1.048E+03
** BCC_A2
    FCC_A1
Calculated            26 equilibria

Phase region boundary 29 at:  3.417E-03  1.048E+03
** BCC_A2
    FCC_A1
Calculated.           16 equilibria
Terminating at known equilibrium

Phase region boundary 30 at:  6.583E-03  9.981E+02
** BCC_A2
    FCC_A1
Calculated            38 equilibria

Phase region boundary 31 at:  6.583E-03  9.981E+02
** BCC_A2
    FCC_A1
Calculated.           3 equilibria
Terminating at known equilibrium

Phase region boundary 32 at:  9.750E-03  1.095E+03
** CEMENTITE
    FCC_A1
Calculated.           12 equilibria
Terminating at known equilibrium

Phase region boundary 33 at:  9.750E-03  1.095E+03
** CEMENTITE
    FCC_A1
Calculated..           3 equilibria
Terminating at known equilibrium
Terminating at axis limit.
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex23\tcex
23a.POLY3
CPU time for mapping          8 seconds
POLY_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

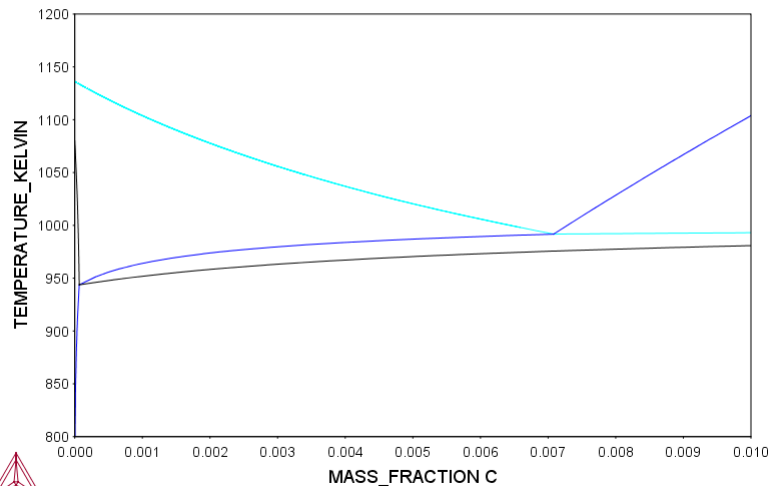
Setting automatic diagram axes

POST:
POST: set-title example 23a
POST: plot

```

... the command in full is PLOT DIAGRAM  
**example 23a**

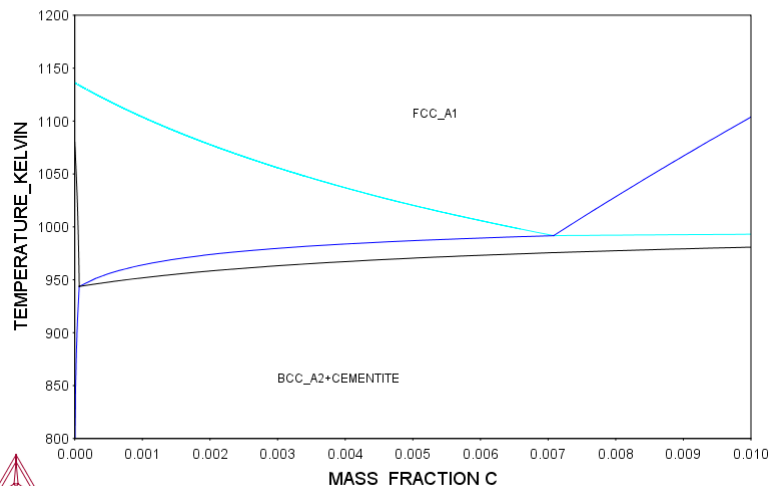
2016.05.16.13.50.27  
 TCFE7: C, FE, MN, SI  
 W(MN)=1.5E-2, W(SI)=3E-3, P=1E5, N=1



POST:  
 POST:Hit RETURN to continue  
 POST: @@ Add labels  
 POST: add  
 ... the command in full is ADD\_LABEL\_TEXT  
 Give X coordinate in axis units: .005  
 Give Y coordinate in axis units: 1100  
 Automatic phase labels? /Y/: Y  
 Automatic labelling not always possible  
 Using global minimization procedure  
 Calculated 15897 grid points in 0 s  
 Found the set of lowest grid points in 0 s  
 Calculated POLY solution 1 s, total time 1 s  
 Stable phases are: FCC\_A1  
 Text size: /.36/. .34  
 POST: add  
 ... the command in full is ADD\_LABEL\_TEXT  
 Give X coordinate in axis units: .003  
 Give Y coordinate in axis units: 850  
 Automatic phase labels? /Y/: Y  
 Automatic labelling not always possible  
 Using global minimization procedure  
 Calculated 15897 grid points in 0 s  
 Found the set of lowest grid points in 0 s  
 Calculated POLY solution 0 s, total time 0 s  
 Stable phases are: BCC\_A2+CEMENTITE  
 Text size: /.36/. .34  
 POST: set-title example 23b  
 POST:  
 POST: plot  
 ... the command in full is PLOT DIAGRAM

**example 23b**

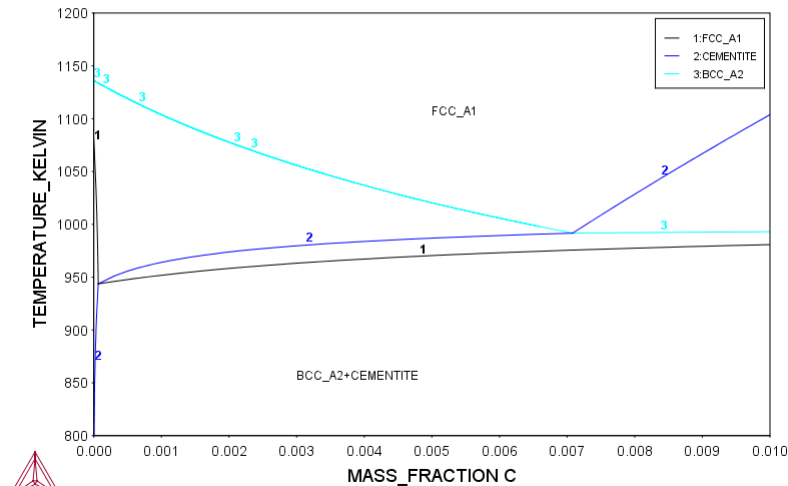
2016.05.16.13.50.29  
 TCFE7: C, FE, MN, SI  
 W(MN)=1.5E-2, W(SI)=3E-3, P=1E5, N=1



POST:  
 POST:Hit RETURN to continue  
 POST: s-lab  
 ... the command in full is SET\_LABEL\_CURVE\_OPTION  
 CURVE LABEL OPTION (A, B, C, D, E, F OR N) /N/: ?  
 THE OPTIONS MEANS:  
 A LIST STABLE PHASES ALONG LINE  
 B AS A BUT CURVES WITH SAME FIX PHASE HAVE SAME NUMBER  
 C LIST AXIS QUANTITIES  
 D AS C BUT CURVES WITH SAME QUANTITIES HAVE SAME NUMBER  
 E AS B WITH CHANGING COLORS  
 F AS D WITH CHANGING COLORS  
 N NO LABELS  
 CURVE LABEL OPTION (A, B, C, D, E, F OR N) /N/: e  
 POST: set-title example 23c  
 POST:

POST: plot  
 ... the command in full is PLOT DIAGRAM  
**example 23c**

2016.05.16.13.50.29  
 TCFe7: C, Fe, Mn, Si  
 W(MN)=1.5E-2, W(Si)=3E-3, P=1E5, N=1



POST:  
 POST:Hit RETURN to continue  
 POST: ba  
 ... the command in full is BACK  
 POLY\_3: @@ Now calculate the T-zero temperature for the steel  
 POLY\_3: read tcex23a  
 ... the command in full is READ\_WORKSPACES  
 POLY\_3: advanced-options  
 Which option? /STEP\_AND\_MAP/: ?  
 EQUILIBRIUM\_CALCUL NEW\_COMPOSITION\_SET SHOW FOR T=  
 GLOBAL\_MINIMIZATION OUTPUT\_FILE\_FOR\_SHOW STABILITY\_CHECK  
 IGNORE\_COMPOSITION\_ORDER PARAEQUILIBRIUM STEP\_AND\_MAP  
 LIST\_PHASE\_ADDITION PHASE\_ADDITION T-ZERO TEMPERATURE  
 MAJOR\_CONSTITUENTS PRESENT\_PHASE TOGGLE\_ALTERNATE\_MODE  
 Which option? /STEP\_AND\_MAP/: t-z

This command calculates the temperature when two phases have the same Gibbs energy. You must calculate an equilibrium at an estimated temperature first.

Name of first phase: fcc  
 Name of second phase: bcc

The T0 temperature is 922.21 K  
 Note: LIST-EQUILIBRIUM is not relevant  
 POLY\_3:Hit RETURN to continue  
 POLY\_3: @@ Calculate the T-zero line, remove the T-axis  
 POLY\_3: l-ax  
 ... the command in full is LIST\_AXIS\_VARIABLE  
 Axis No 1: W(C) Min: 0 Max: 1E-2 Inc: 2.5E-4  
 Axis No 2: T Min: 800 Max: 1200 Inc: 30  
 POLY\_3: s-a-v 2 none  
 ... the command in full is SET\_AXIS\_VARIABLE  
 POLY\_3: save tcex23b y  
 ... the command in full is SAVE\_WORKSPACES  
 POLY\_3: step  
 ... the command in full is STEP\_WITH\_OPTIONS  
 Option? /NORMAL/: ?  
 The following options are available:  
 NORMAL Stepping with given conditions  
 INITIAL\_EQUILIBRIA An initial equilibrium stored at every step  
 EVALUATE Specified variables evaluated after each step  
 SEPARATE\_PHASES Each phase calculated separately  
 T-ZERO T0 line calculation  
 PARAEQUILIBRIUM Paraequilibrium diagram  
 MIXED\_SCHEIL Scheil with fast diffusing elements  
 ONE\_PHASE\_AT\_TIME One phase at a time  
 Option? /NORMAL/: t-z  
 Name of first phase: fcc  
 Name of second phase: bcc

Phase Region from 0.300000E-02 for:  
 BCC\_A2  
 FCC\_A1  
 3.000000E-03 922.21  
 2.750000E-03 932.54  
 2.500000E-03 943.23  
 2.250000E-03 954.34  
 2.000000E-03 965.98  
 1.750000E-03 978.31  
 1.500000E-03 991.57  
 1.250000E-03 1006.14  
 1.000000E-03 1022.76  
 7.500000E-04 1041.59  
 5.000000E-04 1062.86  
 2.500000E-04 1087.12  
 2.500000E-10 1115.11

Phase Region from 0.167112E-02 for:  
 BCC\_A2  
 FCC\_A1  
 1.671124E-03 982.32  
 1.921124E-03 969.73  
 2.171124E-03 957.89  
 2.421124E-03 946.63  
 2.671124E-03 935.82  
 2.921124E-03 925.38  
 3.171124E-03 915.26  
 3.421124E-03 905.40  
 3.671124E-03 895.77  
 3.921124E-03 886.33

```

4.171124E-03      877.06
4.421124E-03      867.93
4.671124E-03      858.95
4.921124E-03      850.07
5.171124E-03      841.30
5.421124E-03      832.63
5.671124E-03      824.03
5.921124E-03      815.51
6.171124E-03      807.06
6.421124E-03      798.67
6.671124E-03      790.33
6.921124E-03      782.04
7.171124E-03      773.79
7.421124E-03      765.58
7.671124E-03      757.40
7.921124E-03      749.26
8.171124E-03      741.14
8.421124E-03      733.04
8.671124E-03      724.96
8.921124E-03      716.90
9.171124E-03      708.85
9.421124E-03      700.82
9.671124E-03      692.79
9.921124E-03      684.77
1.000000E-02      682.24
*** Buffer savend on file
c:\jenkins\WORKSP~1\THERMO~1\examples\tcex23\TCEX23~2.POL
POLY_3: post

```

POLY-3 POSTPROCESSOR VERSION 3.2

```

POST:
POST: set-title example 23d
POST: s-d-a x w(c)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t-k
... the command in full is SET_DIAGRAM_AXIS
POST:
POST: plot
... the command in full is PLOT DIAGRAM

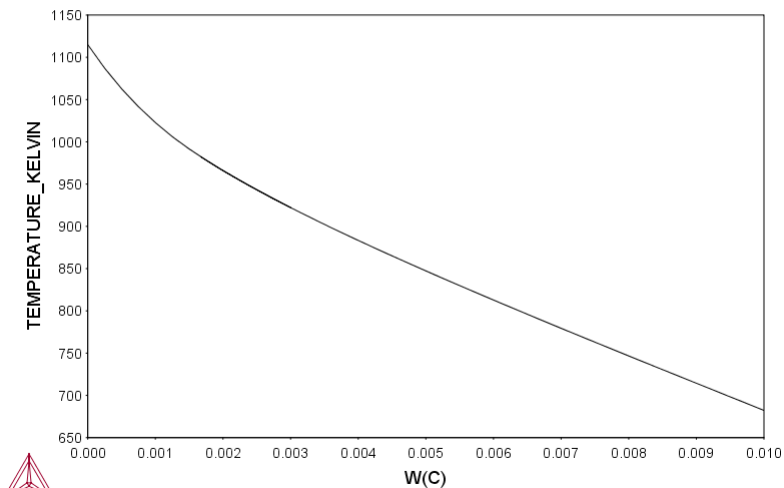
```

example 23d

```

2016.05.16.13.50.35
TCFE7: C, FE, MN, SI
T=682.239, W(MN)=1.502E-2, W(SI)=3.004E-3, P=1E5, N=0.993897

```



```

POST:
POST:Hit RETURN to continue
POST: @@ write the line on a data file
POST: make tcex23b y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: ba
... the command in full is BACK
POLY_3: @@ plot together with phase diagram
POLY_3: read tcex23a
... the command in full is READ_WORKSPACES
POLY_3: post

```

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

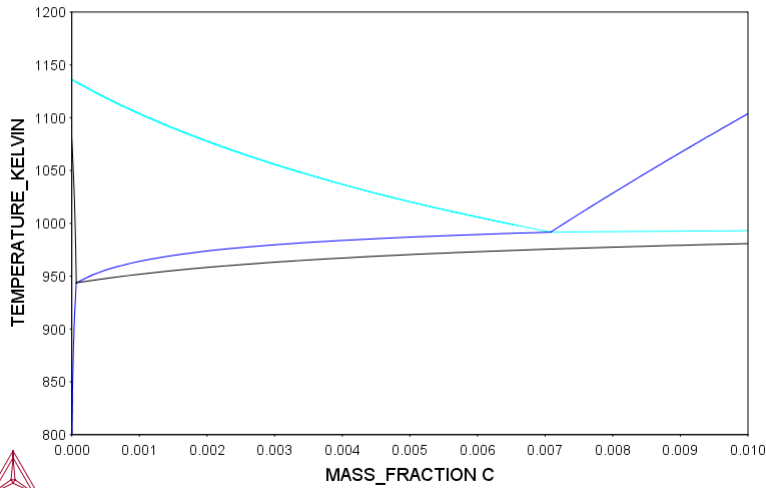
```

POST:
POST: set-title example 23e
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

# example 23e

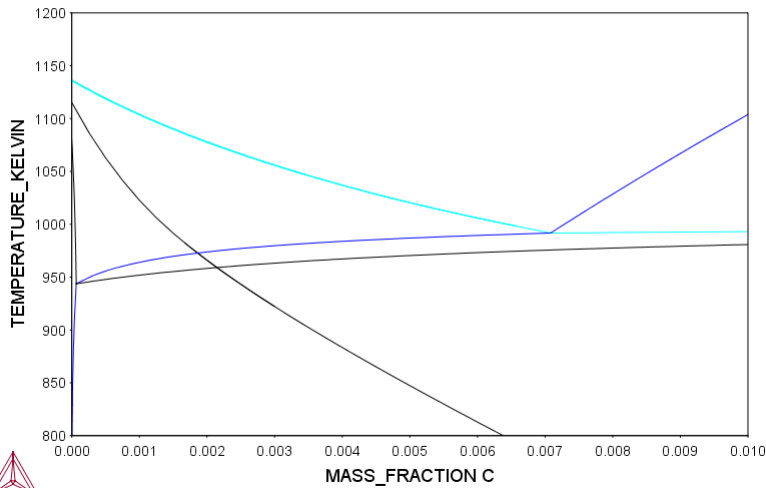
2016.05.16.13.50.35  
TCFE7: C, FE, MN, SI  
W(MN)=1.5E-2, W(SI)=3E-3, P=1E5, N=1



POST:  
POST:Hit RETURN to continue  
POST: a-e-d y tcex23b  
... the command in full is APPEND\_EXPERIMENTAL\_DATA  
PROLOGUE NUMBER: /0/: 0  
DATASET NUMBER(s): /-1/: 1  
POST: set-title example 23f  
POST:  
POST: plot  
... the command in full is PLOT DIAGRAM

## example 23f

2016.05.16.13.50.36  
TCFE7: C, FE, MN, SI  
W(MN)=1.5E-2, W(SI)=3E-3, P=1E5, N=1



POST:  
POST:Hit RETURN to continue  
POST: ba  
... the command in full is BACK  
POLY\_3: @@ Now calculate the para-equilibrium for the steel  
POLY\_3: @@ At paraequilibrium only C is mobile, the other alloying elements have  
POLY\_3: @@ the same compositions in both phases  
POLY\_3: read tcex23a  
... the command in full is READ\_WORKSPACES  
POLY\_3: c-e  
... the command in full is COMPUTE\_EQUILIBRIUM  
Using global minimization procedure  
Calculated 15897 grid points in 0 s  
Found the set of lowest grid points in 0 s  
Calculated POLY solution 0 s, total time 0 s  
POLY\_3: l-e,,,,,  
... the command in full is LIST\_EQUILIBRIUM  
Output from POLY-3, equilibrium = 1, label A0 , database: TCFE7

Conditions:  
T=973.15, W(MN)=1.5E-2, W(SI)=3E-3, W(C)=3E-3, P=1E5, N=1  
DEGREES OF FREEDOM 0

Temperature 973.15 K ( 700.00 C), Pressure 1.000000E+05  
Number of moles of components 1.00000E+00, Mass in grams 5.50671E+01  
Total Gibbs energy -4.16068E+04, Enthalpy 2.38034E+04, Volume 7.22424E-06

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
C	1.3754E-02	3.0000E-03	2.3682E-01	-1.1655E+04	SER
FE	9.6533E-01	9.7900E-01	6.6051E-03	-4.0617E+04	SER
MN	1.5035E-02	1.5000E-02	6.2466E-05	-7.8331E+04	SER
SI	5.8820E-03	3.0000E-03	2.1440E-10	-1.8014E+05	SER

BCC\_A2 Status ENTERED Driving force 0.0000E+00  
Moles 7.6441E-01, Mass 4.2529E+01, Volume fraction 7.7288E-01 Mass fractions:  
FE 9.88221E-01 MN 8.40073E-03 SI 3.26359E-03 C 1.14706E-04

FCC\_A1 Status ENTERED Driving force 0.0000E+00

```

Moles 2.0669E-01, Mass 1.1242E+01, Volume fraction 2.0306E-01 Mass fractions:
FE 9.59011E-01 MN 3.21007E-02 C 6.54001E-03 SI 2.34865E-03

CEMENTITE Status ENTERED Driving force 0.0000E+00
Moles 2.8906E-02, Mass 1.2957E+00, Volume fraction 2.4065E-02 Mass fractions:
FE 8.49786E-01 MN 8.32277E-02 C 6.69864E-02 SI 4.69914E-13
POLY_3: advance para
... the command in full is ADVANCED_OPTIONS

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc
Name of second phase: bcc
Fast diffusing component: /C/: c
Fast diffusing component: /NONE/:
NP(FCC) = 0.4280 with U-fractions C = 3.17220E-02
NP(BCC) = 0.5720 with U-fractions C = 6.47538E-04
All other compositions the same in both phases
Note: LIST-EQUILIBRIUM is not relevant
POLY_3:
POLY_3:Hit RETURN to continue
POLY_3:
POLY_3:
POLY_3: @@ Now calculate the para-equilibrium for the steel at varying temperatures
POLY_3: s-a-v 1 t 800 1200 20
... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 none
... the command in full is SET_AXIS_VARIABLE
POLY_3: save tcex23c y
... the command in full is SAVE_WORKSPACES
POLY_3: step para
... the command in full is STEP_WITH_OPTIONS

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc
Name of second phase: bcc
Fast diffusing component: /C/: c
Fast diffusing component: /NONE/:
Output during stepping is:
axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,
and LNACR value(s) of interstitial(s)

Phase Region from 973.150 for:
BCC_A2
FCC_A1
9.731500E+02 0.428 0.572 3.172200E-02 6.475377E-04 -1.290452E+00
9.531500E+02 0.345 0.655 3.908052E-02 7.297760E-04 -8.659516E-01
9.331500E+02 0.285 0.715 4.699458E-02 8.039957E-04 -4.522834E-01
9.131500E+02 0.240 0.760 5.535054E-02 8.679372E-04 -4.631426E-02
8.931500E+02 0.206 0.794 6.405501E-02 9.201210E-04 3.549783E-01
8.731500E+02 0.180 0.820 7.303132E-02 9.596491E-04 7.543208E-01
8.531500E+02 0.160 0.840 8.221743E-02 9.860983E-04 1.154160E+00
8.331500E+02 0.143 0.857 9.156332E-02 9.994314E-04 1.556708E+00
8.131500E+02 0.129 0.871 1.010286E-01 9.999336E-04 1.963997E+00
8.000000E+02 0.122 0.878 1.073012E-01 9.935324E-04 2.235299E+00

Phase Region from 973.150 for:
BCC_A2
FCC_A1
9.731500E+02 0.429 0.571 3.168117E-02 6.465368E-04 -1.292139E+00
9.931500E+02 0.547 0.453 2.501532E-02 5.595693E-04 -1.730355E+00
1.013150E+03 0.720 0.280 1.919684E-02 4.725723E-04 -2.182535E+00
1.033150E+03 0.977 0.023 1.426175E-02 3.879729E-04 -2.653059E+00
1.053150E+03 1.411 -0.411 9.973814E-03 3.003908E-04 -3.172815E+00
1.073150E+03 2.275 -1.275 6.247344E-03 2.085287E-04 -3.792875E+00
1.093150E+03 4.762 -3.762 3.016699E-03 1.116447E-04 -4.664306E+00
1.113150E+03 64.105 -63.105 2.267080E-04 9.302453E-06 -7.388093E+00
*** Buffer savend on file
c:\jenkins\WORKSP~1\THERMO~1\examples\tcex23\TCEx23~3.POL

*** ERROR 7 IN NS01AD
*** Numerical error
POLY_3:
POLY_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

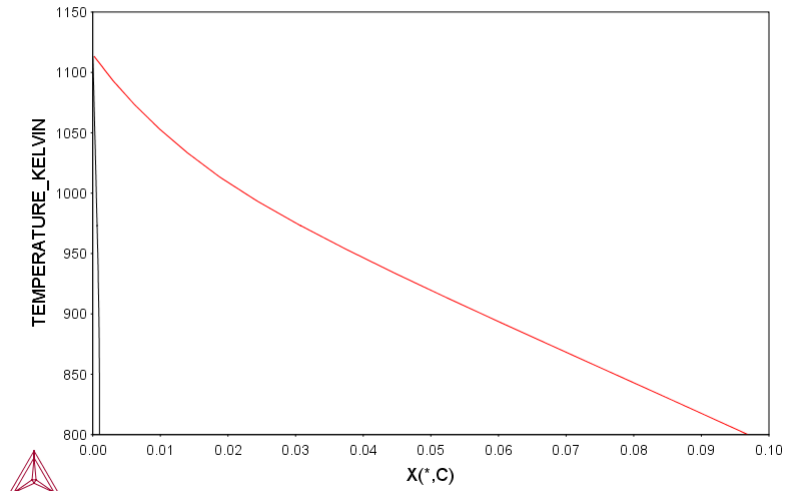
Setting automatic diagram axes

POST:
POST:
POST: set-title example 23g
POST: s-d-a x (*,c)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: s-d-a y t-k
... the command in full is SET_DIAGRAM_AXIS
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

### example 23g

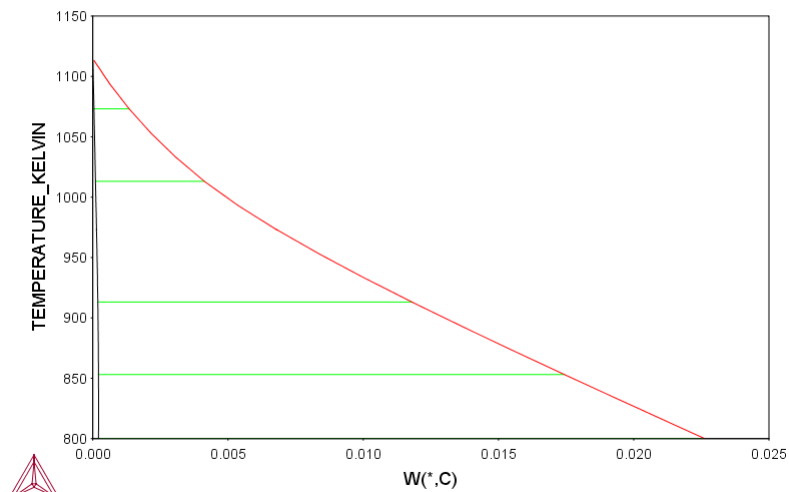
2016.05.16.13.50.39  
TCFE7: C, FE, MN, SI  
W(MN)=1.50451E-2, W(SI)=3.00903E-3, W(C)=3.00903E-3, P=1E5, N=1.



```
POST:
POST:Hit RETURN to continue
POST: s-d-a x w(*,c)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST:
POST: s-t-s 3
... the command in full is SET_TIELINE_STATUS
POST: set-title example 23h
POST:
POST: plot
... the command in full is PLOT DIAGRAM
```

### example 23h

2016.05.16.13.50.39  
TCFE7: C, FE, MN, SI  
W(MN)=1.50451E-2, W(SI)=3.00903E-3, W(C)=3.00903E-3, P=1E5, N=1.



```
POST:
POST:Hit RETURN to continue
POST: make tcex23c y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: ba
... the command in full is BACK
POLY_3: read tcex23a
... the command in full is READ_WORKSPACES
POLY_3: post
```

POLY-3 POSTPROCESSOR VERSION 3.2

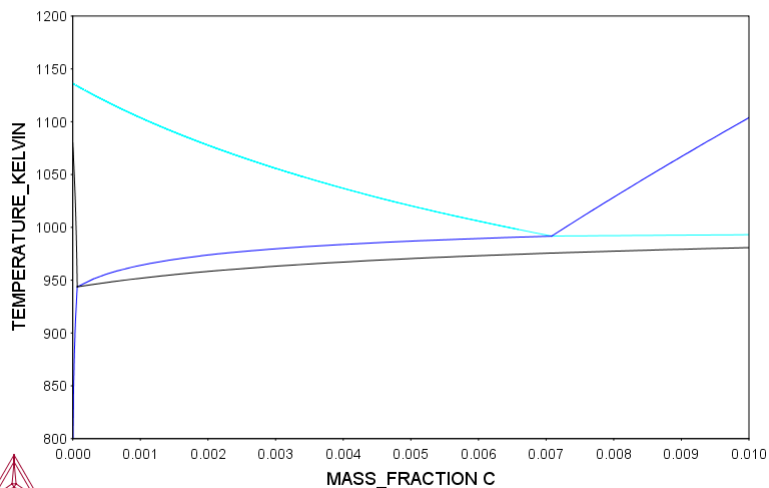
Setting automatic diagram axes

```
POST:
POST:
POST: set-title example 23i
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
```



# example 23i

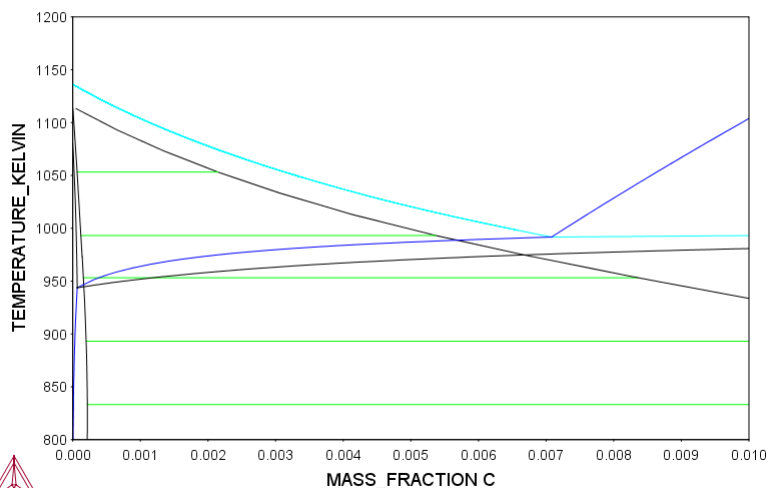
2016.05.16.13.50.39  
TCFE7: C, FE, MN, SI  
W(MN)=1.5E-2, W(SI)=3E-3, P=1E5, N=1



POST:  
POST:Hit RETURN to continue  
POST: a-e-d y tcex23c  
... the command in full is APPEND\_EXPERIMENTAL\_DATA  
PROLOGUE NUMBER: /0/: 0  
DATASET NUMBER(s): /-1/: 1  
POST: set-title example 23j  
POST:  
POST: plot  
... the command in full is PLOT DIAGRAM

# example 23j

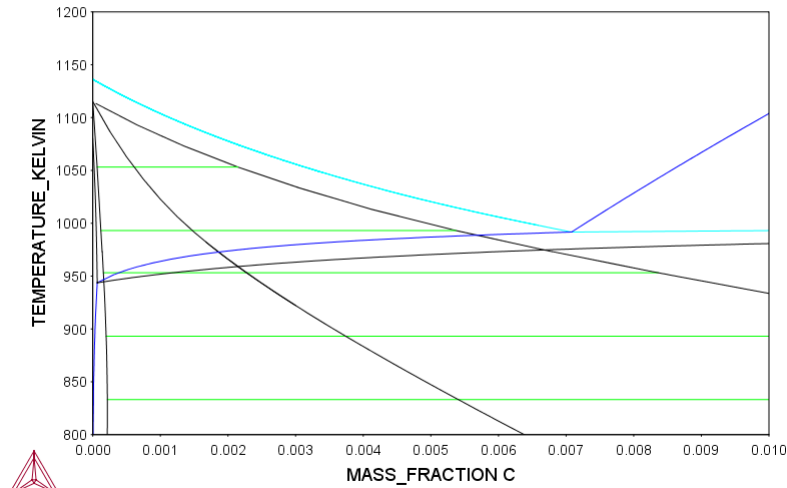
2016.05.16.13.50.40  
TCFE7: C, FE, MN, SI  
W(MN)=1.5E-2, W(SI)=3E-3, P=1E5, N=1



POST:  
POST:Hit RETURN to continue  
POST: a-e-d y tcex23b.exp tcex23c.exp 0; 1; 0; 1;  
... the command in full is APPEND\_EXPERIMENTAL\_DATA  
POST:  
POST: set-title example 23k  
POST:  
POST: plot  
... the command in full is PLOT\_DIAGRAM

# example 23k

2016.05.16.13.50.40  
TCFE7: C, FE, MN, SI  
W(MN)=1.5E-2, W(SI)=3E-3, P=1E5, N=1



```
POST:
POST:Hit RETURN to continue
POST: ba
... the command in full is BACK
POLY_3: @@ Now calculate both a normal and para-equilibrium for the steel at 1000 K
POLY_3: @@ Note that a para equilibrium does not always exist for the given conditions
POLY_3: @@ The calculated results are the amounts of the two phases.
POLY_3: @@ This indicates how much of the phases that can be transformed
POLY_3: @@ at para-equilibrium conditions.
POLY_3: @@ The carbon content of the phases are also listed,
POLY_3: @@ the other alloying elements have the same fractions in both phases
POLY_3: read tcex23a.POLY3
... the command in full is READ_WORKSPACES
POLY_3: s-c T=1000
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      15897 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution      0 s, total time    0 s
POLY_3: l-e,,,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium =      1, label A0 , database: TCFE7
```

Conditions:  
T=1000, W(MN)=1.5E-2, W(SI)=3E-3, W(C)=3E-3, P=1E5, N=1  
DEGREES OF FREEDOM 0

Temperature 1000.00 K ( 726.85 C), Pressure 1.000000E+05  
Number of moles of components 1.000000E+00, Mass in grams 5.50671E+01  
Total Gibbs energy -4.34548E+04, Enthalpy 2.63172E+04, Volume 7.20607E-06

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
C	1.3754E-02	3.0000E-03	1.6744E-01	-1.4859E+04	SER
FE	9.6533E-01	9.7900E-01	6.1057E-03	-4.2392E+04	SER
MN	1.5035E-02	1.5000E-02	4.1161E-05	-8.3960E+04	SER
SI	5.8820E-03	3.0000E-03	3.4194E-10	-1.8123E+05	SER

FCC A1 Status ENTERED Driving force 0.0000E+00  
Moles 5.3820E-01, Mass 2.9381E+01, Volume fraction 5.3141E-01 Mass fractions:  
FE 9.69754E-01 MN 2.22121E-02 C 5.51915E-03 SI 2.51464E-03

BCC A2 Status ENTERED Driving force 0.0000E+00  
Moles 4.6180E-01, Mass 2.5686E+01, Volume fraction 4.6859E-01 Mass fractions:  
FE 9.89576E-01 MN 6.75038E-03 SI 3.55518E-03 C 1.18465E-04

```
POLY_3: advanced
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: para
```

This command calculates a paraequilibrium between two phases.  
You must calculate an equilibrium with the overall composition first.

```
Name of first phase: fcc
Name of second phase: bcc
Fast diffusing component: /C/: c
Fast diffusing component: /NONE/:
```

NP(FCC) = 0.5982 with U-fractions C = 2.29562E-02  
NP(BCC) = 0.4018 with U-fractions C = 5.30475E-04  
All other compositions the same in both phases  
Note: LIST-EQUILIBRIUM is not relevant

```
POLY_3:
POLY_3:Hit RETURN to continue
POLY_3: @@ Now calculate an isothermal phase diagram at 1000 K
POLY_3: s-a-v 2 w(mn) 0 .1,,,
... the command in full is SET_AXIS_VARIABLE
POLY_3:Hit RETURN to continue
POLY_3: save tcex23d y
... the command in full is SAVE_WORKSPACES
POLY_3: map
```

Version S mapping is selected  
Generating start equilibrium 1  
Generating start equilibrium 2  
Generating start equilibrium 3  
Generating start equilibrium 4  
Generating start equilibrium 5  
Generating start equilibrium 6  
Generating start equilibrium 7  
Generating start equilibrium 8  
Generating start equilibrium 9  
Generating start equilibrium 10  
Generating start equilibrium 11

Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Tie-lines not in the plane of calculation

Generating start point 1  
Generating start point 2  
Generating start point 3  
Generating start point 4  
Generating start point 5  
Generating start point 6  
Generating start point 7  
Generating start point 8  
Generating start point 9  
Generating start point 10  
Working hard  
Generating start point 11  
Generating start point 12  
Generating start point 13  
Generating start point 14  
Generating start point 15  
Generating start point 16  
Generating start point 17  
Generating start point 18  
Generating start point 19  
Generating start point 20  
Working hard  
Generating start point 21  
Generating start point 22  
Generating start point 23  
Generating start point 24  
Generating start point 25  
Generating start point 26  
Generating start point 27  
Generating start point 28  
Generating start point 29  
Generating start point 30  
Working hard  
Generating start point 31  
Generating start point 32

Phase region boundary 1 at: 2.585E-03 2.500E-03  
BCC\_A2  
\*\* CEMENTITE  
FCC\_A1  
Calculated. 11 equilibria

Phase region boundary 2 at: 1.821E-04 1.138E-03  
BCC\_A2  
\*\* CEMENTITE  
\*\* FCC\_A1

Phase region boundary 3 at: 1.821E-04 1.138E-03  
BCC\_A2  
\*\* CEMENTITE  
Calculated 14 equilibria

Phase region boundary 4 at: 1.821E-04 1.138E-03  
BCC\_A2  
\*\* FCC\_A1  
Calculated 24 equilibria

Phase region boundary 5 at: 1.821E-04 1.138E-03  
BCC\_A2  
CEMENTITE  
\*\* FCC\_A1  
Calculated.. 41 equilibria  
Terminating at axis limit.

Phase region boundary 6 at: 1.821E-04 1.138E-03  
BCC\_A2  
\*\* CEMENTITE  
FCC\_A1  
Calculated. 30 equilibria

Phase region boundary 7 at: 7.345E-03 6.913E-03  
\*\* BCC\_A2  
\*\* CEMENTITE  
FCC\_A1

Phase region boundary 8 at: 7.345E-03 6.913E-03  
\*\* CEMENTITE  
FCC\_A1  
Calculated.. 39 equilibria  
Terminating at axis limit.

Phase region boundary 9 at: 7.345E-03 6.913E-03  
\*\* BCC\_A2  
FCC\_A1  
Calculated 40 equilibria

Phase region boundary 10 at: 7.345E-03 6.913E-03  
\*\* BCC\_A2  
CEMENTITE  
FCC\_A1  
Calculated.. 13 equilibria  
Terminating at axis limit.

Phase region boundary 11 at: 2.585E-03 2.500E-03  
BCC\_A2  
\*\* CEMENTITE  
FCC\_A1  
Calculated. 21 equilibria  
Terminating at known equilibrium

Phase region boundary 12 at: 2.500E-04 5.813E-02  
\*\* BCC\_A2  
FCC\_A1  
Calculated 22 equilibria

Phase region boundary 13 at: 2.500E-04 5.813E-02  
\*\* BCC\_A2  
FCC\_A1  
Calculated. 30 equilibria

Terminating at known equilibrium

Phase region boundary 14 at: 3.417E-03 3.078E-03  
 BCC\_A2  
 \*\* CEMENTITE  
 FCC\_A1  
 Calculated. 14 equilibria  
 Terminating at known equilibrium

Phase region boundary 15 at: 3.417E-03 3.078E-03  
 BCC\_A2  
 \*\* CEMENTITE  
 FCC\_A1  
 Calculated. 17 equilibria  
 Terminating at known equilibrium

Phase region boundary 16 at: 6.583E-03 5.991E-03  
 BCC\_A2  
 \*\* CEMENTITE  
 FCC\_A1  
 Calculated. 27 equilibria  
 Terminating at known equilibrium

Phase region boundary 17 at: 6.583E-03 5.991E-03  
 BCC\_A2  
 \*\* CEMENTITE  
 FCC\_A1  
 Calculated. 5 equilibria  
 Terminating at known equilibrium

Phase region boundary 18 at: 7.601E-03 2.500E-03  
 BCC\_A2  
 CEMENTITE  
 \*\* FCC\_A1  
 Calculated. 31 equilibria  
 Terminating at known equilibrium

Phase region boundary 19 at: 7.601E-03 2.500E-03  
 BCC\_A2  
 CEMENTITE  
 \*\* FCC\_A1  
 Calculated.. 11 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 20 at: 9.750E-03 2.959E-03  
 BCC\_A2  
 CEMENTITE  
 \*\* FCC\_A1  
 Calculated. 40 equilibria  
 Terminating at known equilibrium

Phase region boundary 21 at: 9.750E-03 2.959E-03  
 BCC\_A2  
 CEMENTITE  
 \*\* FCC\_A1  
 Calculated.. 3 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 22 at: 4.016E-03 3.417E-02  
 \*\* BCC\_A2  
 FCC\_A1  
 Calculated. 22 equilibria  
 Terminating at known equilibrium

Phase region boundary 23 at: 4.016E-03 3.417E-02  
 \*\* BCC\_A2  
 FCC\_A1  
 Calculated 33 equilibria

Phase region boundary 24 at: 7.141E-03 3.417E-02  
 \*\* CEMENTITE  
 FCC\_A1  
 Calculated. 12 equilibria  
 Terminating at known equilibrium

Phase region boundary 25 at: 7.141E-03 3.417E-02  
 \*\* CEMENTITE  
 FCC\_A1  
 Calculated.. 28 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 26 at: 6.924E-03 6.583E-02  
 \*\* CEMENTITE  
 FCC\_A1  
 Calculated. 25 equilibria  
 Terminating at known equilibrium

Phase region boundary 27 at: 6.924E-03 6.583E-02  
 \*\* CEMENTITE  
 FCC\_A1  
 Calculated.. 15 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 28 at: 6.924E-03 6.583E-02  
 \*\* CEMENTITE  
 FCC\_A1  
 Calculated. 25 equilibria  
 Terminating at known equilibrium

Phase region boundary 29 at: 6.924E-03 6.583E-02  
 \*\* CEMENTITE  
 FCC\_A1  
 Calculated.. 15 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 30 at: 6.732E-03 9.750E-02  
 \*\* CEMENTITE  
 FCC\_A1  
 Calculated. 38 equilibria  
 Terminating at known equilibrium

```

Phase region boundary 31 at: 6.732E-03 9.750E-02
** CEMENTITE
FCC_A1
Calculated.. 3 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 32 at: 2.500E-04 5.813E-02
** BCC_A2
FCC_A1
Calculated 4 equilibria

Phase region boundary 33 at: 2.500E-04 5.813E-02
** BCC_A2
FCC_A1
Calculated. 30 equilibria
Terminating at known equilibrium

Phase region boundary 34 at: 3.417E-03 3.841E-02
** BCC_A2
FCC_A1
Calculated 26 equilibria

Phase region boundary 35 at: 3.417E-03 3.841E-02
** BCC_A2
FCC_A1
Calculated. 17 equilibria
Terminating at known equilibrium

Phase region boundary 36 at: 6.583E-03 1.374E-02
** BCC_A2
FCC_A1
Calculated 38 equilibria

Phase region boundary 37 at: 6.583E-03 1.374E-02
** BCC_A2
FCC_A1
Calculated. 5 equilibria
Terminating at known equilibrium

Phase region boundary 38 at: 6.732E-03 9.750E-02
** CEMENTITE
FCC_A1
Calculated. 38 equilibria
Terminating at known equilibrium

Phase region boundary 39 at: 6.732E-03 9.750E-02
** CEMENTITE
FCC_A1
Calculated.. 3 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 40 at: 9.750E-03 7.619E-03
** BCC_A2
CEMENTITE
FCC_A1
Calculated. 11 equilibria
Terminating at known equilibrium

Phase region boundary 41 at: 9.750E-03 7.619E-03
** BCC_A2
CEMENTITE
FCC_A1
Calculated.. 3 equilibria
Terminating at known equilibrium
Terminating at axis limit.
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex23\tcex
23d.POLY3
CPU time for mapping 5 seconds
POLY_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

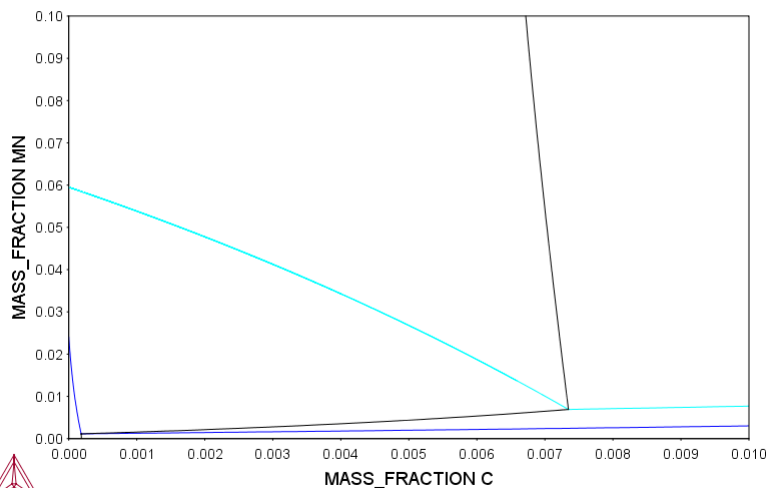
Setting automatic diagram axes

POST:
POST:
POST: set-title example 231
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

### example 23l

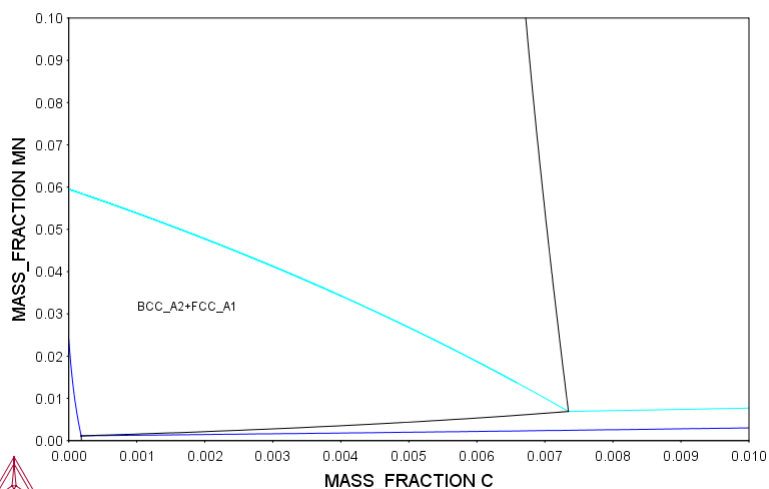
2016.05.16.13.50.48  
TCFE7: C, FE, MN, SI  
T=1000, W(SI)=3E-3, P=1E5, N=1



POST:  
POST:Hit RETURN to continue  
POST: add .001 .03,,,,  
... the command in full is ADD\_LABEL\_TEXT  
Automatic labelling not always possible  
Using global minimization procedure  
Using already calculated grid  
Found the set of lowest grid points in 0 s  
Calculated POLY solution 0 s, total time 0 s  
Stable phases are: BCC\_A2+FCC\_A1  
POST: set-title example\_23m

POST:  
POST: plot  
... the command in full is PLOT DIAGRAM  
example 23m

2016.05.16.13.50.49  
TCFE7: C, FE, MN, SI  
T=1000, W(SI)=3E-3, P=1E5, N=1



POST:  
POST:Hit RETURN to continue  
POST: ba  
... the command in full is BACK  
POLY\_3: @@ Calculate the corresponding para-equilibrium diagram  
POLY\_3: @@ where fcc and bcc have the same alloy composition.  
POLY\_3: read tcex23d  
... the command in full is READ\_WORKSPACES  
POLY\_3: @@ Only one axis is set, the interstitial composition  
POLY\_3: @@ must not be an axis  
POLY\_3: s-a-v 1 w(mn) 0 .1,,,,  
... the command in full is SET\_AXIS\_VARIABLE  
POLY\_3: s-a-v 2 none  
... the command in full is SET\_AXIS\_VARIABLE  
POLY\_3: save tcex23e y  
... the command in full is SAVE\_WORKSPACES  
POLY\_3: step  
... the command in full is STEP\_WITH\_OPTIONS  
Option? /NORMAL/: ?  
The following options are available:  
NORMAL Stepping with given conditions  
INITIAL\_EQUILIBRIA An initial equilibrium stored at every step  
EVALUATE Specified variables evaluated after each step  
SEPARATE\_PHASES Each phase calculated separately  
T-ZERO T0 line calculation  
PARAEQUILIBRIUM Paraequilibrium diagram  
MIXED\_SCHEIL Scheil with fast diffusing elements  
ONE\_PHASE\_AT\_TIME One phase at a time  
Option? /NORMAL/: para

This command calculates a paraequilibrium between two phases.  
You must calculate an equilibrium with the overall composition first.

Name of first phase: fcc  
Name of second phase: bcc

Fast diffusing component: /C/: c  
 Fast diffusing component: /NONE/:  
 Output during stepping is:  
 axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,  
 and LNACR value(s) of interstitial(s)

Phase Region from 0.150000E-01 for:

	BCC_A2	FCC_A1				
1.500000E-02	0.598	0.402	2.295618E-02	5.304752E-04	-1.881771E+00	
1.250000E-02	0.542	0.458	2.524490E-02	5.935358E-04	-1.753638E+00	
1.000000E-02	0.494	0.506	2.753767E-02	6.587191E-04	-1.633619E+00	
7.500000E-03	0.454	0.546	2.983359E-02	7.260508E-04	-1.520467E+00	
5.000000E-03	0.420	0.580	3.213187E-02	7.955567E-04	-1.413204E+00	
2.500000E-03	0.390	0.610	3.443178E-02	8.672626E-04	-1.311054E+00	
2.500000E-09	0.363	0.637	3.673267E-02	9.411946E-04	-1.213385E+00	

Phase Region from 0.150000E-01 for:

	BCC_A2	FCC_A1				
1.500000E-02	0.598	0.402	2.295989E-02	5.306073E-04	-1.881370E+00	
1.750000E-02	0.667	0.333	2.067628E-02	4.696395E-04	-2.019223E+00	
2.000000E-02	0.752	0.248	1.839858E-02	4.107379E-04	-2.169018E+00	
2.250000E-02	0.862	0.138	1.612841E-02	3.538881E-04	-2.333767E+00	
2.500000E-02	1.006	-0.006	1.386691E-02	2.990604E-04	-2.517864E+00	
2.750000E-02	1.205	-0.205	1.161307E-02	2.461731E-04	-2.728233E+00	
3.000000E-02	1.501	-0.501	9.357235E-03	1.949519E-04	-2.977273E+00	
3.250000E-02	1.985	-0.985	7.097179E-03	1.453158E-04	-3.286868E+00	
3.500000E-02	2.925	-1.925	4.831565E-03	9.721155E-05	-3.704636E+00	
3.750000E-02	5.540	-4.540	2.558996E-03	5.058863E-05	-4.373542E+00	
4.000000E-02	51.139	-50.139	2.780008E-04	5.399171E-06	-6.626764E+00	

\*\*\* Buffer savend on file  
 c:\jenkins\WORKSP~1\THERMO~1\examples\tccex23\TC9F56~1.POL

\*\*\* ERROR 8 IN NS01AD  
 \*\*\* Numerical error

POLY\_3:  
 POLY\_3: post

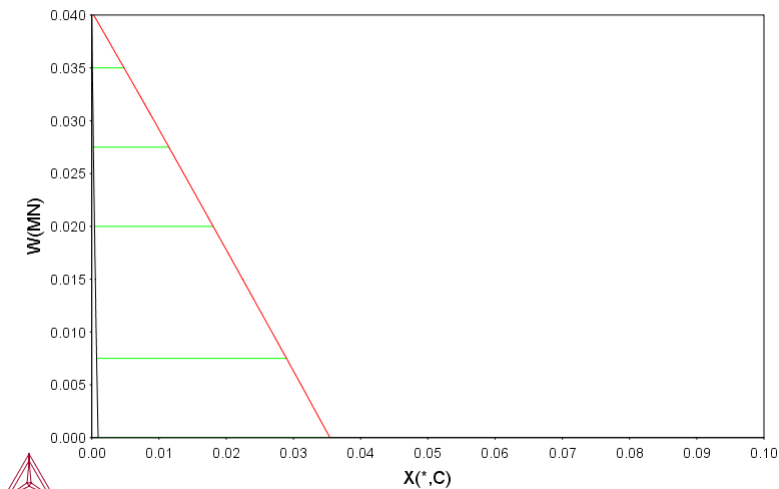
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST:  
 POST:  
 POST: s-t-s 3  
 ... the command in full is SET\_TIELINE\_STATUS  
 POST: set-title example 23n  
 POST:  
 POST: plot  
 ... the command in full is PLOT DIAGRAM

example 23n

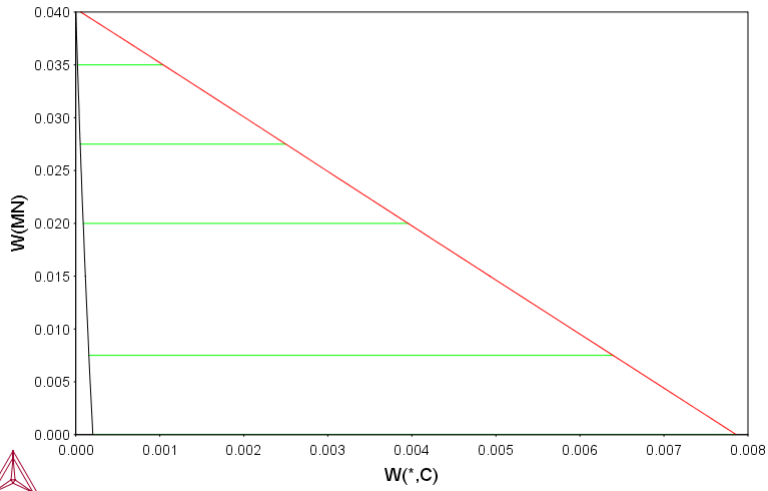
2016.05.16.13.50.51  
 TCFE7: C, FE, MN, SI  
 T=1000, W(SI)=3.00903E-3, W(C)=3.00903E-3, P=1E5, N=1.



POST:  
 POST:Hit RETURN to continue  
 POST: s-d-a x w(\*,c)  
 ... the command in full is SET\_DIAGRAM\_AXIS  
 COLUMN NUMBER /\*/:  
 POST:  
 POST: set-title example 23o  
 POST:  
 POST: plot  
 ... the command in full is PLOT\_DIAGRAM

# example 23o

2016.05.16.13.50.52  
TCFE7: C, FE, MN, SI  
T=1000, W(SI)=3.00903E-3, W(C)=3.00903E-3, P=1E5, N=1.



POST:  
POST: make tcex23e y  
... the command in full is MAKE\_EXPERIMENTAL\_DATAFI  
POST:Hit RETURN to continue  
POST: ba  
... the command in full is BACK  
POLY\_3: @@ Now overlay the two diagrams  
POLY\_3: read tcex23d  
... the command in full is READ\_WORKSPACES  
POLY\_3: post

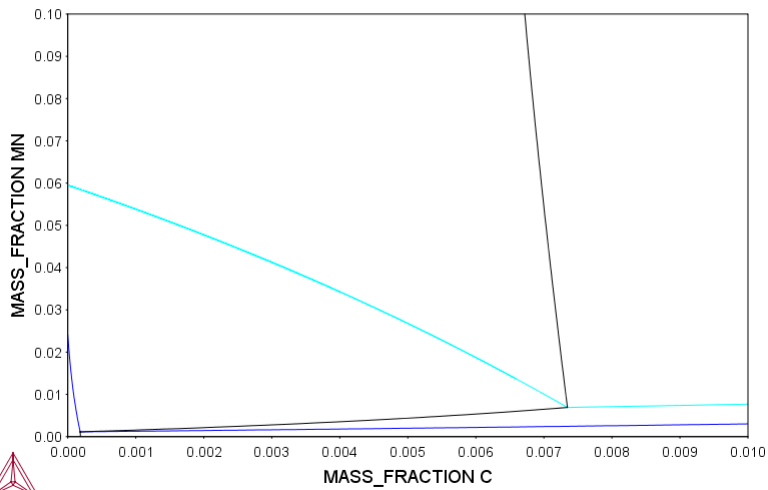
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST:  
POST:  
POST: set-title example 23p  
POST:  
POST: plot  
... the command in full is PLOT DIAGRAM

# example 23p

2016.05.16.13.50.53  
TCFE7: C, FE, MN, SI  
T=1000, W(SI)=3E-3, P=1E5, N=1

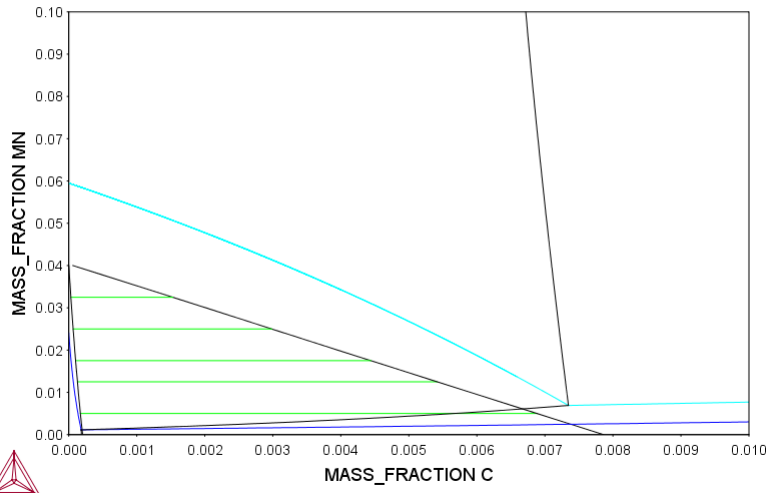


POST:  
POST:Hit RETURN to continue  
POST: a-e-d y tcex23e  
... the command in full is APPEND\_EXPERIMENTAL\_DATA  
PROLOGUE NUMBER: /0/: 0  
DATASET NUMBER(s): /-1/: 1  
POST: set-title example 23q  
POST:  
POST: plot  
... the command in full is PLOT\_DIAGRAM



# example 23q

2016.05.16.13.50.53  
TCFE7: C, FE, MN, SI  
T=1000, W(SI)=3E-3, P=1E5, N=1



POST:  
POST: set-inter  
... the command in full is SET\_INTERACTIVE\_MODE  
POST:

**About**

Software (build 9533) running on WinNT 64-bit wordlength  
 Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118  
 License library version: 8.5.1.0017  
 Linked: Mon May 16 09:31:44 2016

**SYS:** **SYS:** **MACRO** "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex24\tcex24.TCM" set-echo

**SYS:** @@

**SYS:** @@

**SYS:** @@ Simulation of the silicon arc furnace using the REACTOR module

**SYS:** @@

**SYS:** @@ This is a very simple reactor model with output of gases at the top

**SYS:** @@ and output of condensed phases at the bottom. The gas phase from

**SYS:** @@ one segment will flow to higher segments, 80 % will react in the

**SYS:** @@ first above, 15% in the second above and 5 % in the third above.

**SYS:** @@ The condensed phases will flow downwards and all of it will go

**SYS:** @@ to the next lowest segment.

**SYS:** @@ Heat can be added at any module. The only way to specify the

**SYS:** @@ initial state of the reactants added to the reactor is to specify

**SYS:** @@ their heat content.

**SYS:** @@

**SYS:** @@ First fetch data

**SYS:** GO DAT

THERMODYNAMIC DATABASE module

Current database: Steels/Fe-Alloys v8.0

VA DEFINED

L12 FCC

B2\_BCC

B2\_VACANCY

HIGH SIGMA

DICTRA\_FCC\_A1 REJECTED

**TDB\_TCFE8:** SW SSUB5

Current database: SGTE Substances Database v5.1

VA DEFINED

**TDB\_SSUB5:**

**TDB\_SSUB5:** @@ Define-species means that data for just these species will be retrieved

**TDB\_SSUB5:** @@ Define-system would mean that data for all combinations of the elements

**TDB\_SSUB5:** @@ would be retrieved and this is not necessary here.

**TDB\_SSUB5:** DEF-SPECIES C C101 C102 C1Si1 C2 C3 N101 N2 N4Si3

C

C102

C1Si1

C3

N101

N2

N4Si3

DEFINED

**TDB\_SSUB5:** DEF-SP O O2 SI O1Si1 O2Si1

O

O2

SI

O1Si1

O2Si1 DEFINED

**TDB\_SSUB5:** GET

REINITIATING GES5 .....

ELEMENTS .....

SPECIES .....

PHASES .....

PARAMETERS ...

FUNCTIONS ....

List of references for assessed data

C1<G> T.C.R.A.S. Class: 1

C1<G> C<G>

C101<G> JANAF THERMOCHEMICAL TABLES SGTE \*\*

C101<G> CO<G>

CARBON MONOXIDE <GAS>

STANDARD STATE : CODATA KEY VALUE. /CP FROM JANAF PUB. 9/65

C102<G> T.C.R.A.S. Class: 2

C102<G> CO2<G>

CARBON DIOXIDE <GAS>

C1Si1<G> T.C.R.A.S. Class: 5

C1Si1<G> SiC<G>

SILICON CARBIDE <GAS>

C2<G> T.C.R.A.S. Class: 2

C2<G>

CARBON Diatomic Gas.

C3<G> T.C.R.A.S. Class: 6

C3<G>

CARBON <TRIATOMIC GAS>

N101<G> T.C.R.A.S. Class: 1

N101<G> NO<G>

NITRIC OXIDE <GAS>

N2<G> JANAF THERMOCHEMICAL TABLES SGTE \*\*

N2<G> N2<G>

NITROGEN <DIATOMIC GAS>

PUBLISHED BY JANAF AT 09/65

O1<G> TCRAS 02/06/80

O1<G> O<G>

O1Si1<G> T.C.R.A.S. Class: 1

O1Si1<G> SiO<G>

SILICON <MONOXIDE GAS>

O2<G> TCRAS 21/06/90

O2<G>

OXYGEN Gaseous Standard State.

O2Si1<G> T.C.R.A.S. Class: 5

O2Si1<G> SiO2<G>

SILICON DIOXIDE <GAS>

Si1<G> T.C.R.A.S. Class: 1

Si1<G> Si<G>

SILICON <GAS>

O2Si1<BETA-QUARTZ> N.P.L.

O2Si1\_BETA\_QUARTZ SiO2\_BETA\_QUARTZ

Data from an assessment by T I Barry, reported in paper on CaO-SiO2

system by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88

C1Si1<C1Si1\_ALPHA> JANAF THERMOCHEMICAL TABLES SGTE \*\*

C1Si1\_ALPHA SiC\_ALPHA

N CARBIDE <ALPHA>

ALPHA-SiC . HEX.FORM . PUBL. BY JANAF AT 3/67 .LESS STABLE THAN

SiC\_BETA UP TO 2200K. Decomposes to complex vapour at about 3259K.

C1Si1<C1Si1\_BETA> JANAF THERMOCHEMICAL TABLES SGTE

C1Si1\_BETA SiC\_BETA

N CARBIDE <BETA>

CUBIC FORM OF TYPE ZNS. STABLE WITH RESPECT TO SiC-ALPHA UP TO 2200K.

PUBL. BY JANAF 03/67

O2Si1<CRISTOBALITE> N.P.L.

O2Si1\_CRISTOBALITE SiO2\_CRISTOBALITE

Data from an assessment by T I Barry, reported in paper on CaO-SiO2  
syst  
by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88  
C1<DIAMOND> S.G.T.E. \*\*  
C DIAMOND  
<DIAMOND>  
Data from SGTE Unary DB, data added by atd 7/9/95, H298-H0 taken  
from 1994 database (ex THERMODATA 01/93)  
C1<GRAPHITE> S.G.T.E. \*\*  
C GRAPHITE  
Data from SGTE Unary DB, pressure dependent data added by atd 7/9/95  
N4SI3 CHATILLON(1997)  
N4SI3 Si3N4  
Gurvich V.V., Veyts I.V., Alcock C.B., Thermodynamical Properties of  
Individual Substances, 4th ed. Vol 1 and 2 English Ed (1990). S(298)  
corrected according to Koshchenko V.I., Grindberg Ya. Zh. Inorg.  
Mater.  
18(6) 903-5 (1982). Recent calorimetric determination par O'Hare et  
al., J. Mater. Res., 12 (1997) 3203-3205. Enthalpy of transformation  
alpha to beta very small(1 +- 4 kJ/ mol ) but no knowledge of T trans.  
according to them.  
O2SI1<QUARTZ> N.P.L.  
O2SI1\_QUARTZ SiO2\_Quartz  
Data from an assessment by T I Barry, reported in paper on CaO-SiO2  
syst  
by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88  
O2SI1<SiO2 LIQUID> N.P.L.  
O2SI1\_LIQUID SiO2\_Liquid  
Data from an assessment by T I Barry, reported in paper on CaO-SiO2  
syst  
by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88  
SI1 JANAF THERMOCHEMICAL TABLES SGTE \*\*  
SI1 Si  
SILICON  
PUBLISHED BY JANAF AT 12/66 . MPT FROM NBS BULL. (IPTS-68)  
--U.D. 31/10/85  
O2SI1<TRIDYMIT> N.P.L.  
O2SI1\_TRIDYMIT SiO2\_TRIDYMIT  
Data from an assessment by T I Barry, reported in paper on CaO-SiO2  
syst  
by J R Taylor and A T Dinsdale, CALPHAD, 1990, 19(1), 71-88

-OK-

TDB\_SSUB5: GO G

GIBBS ENERGY SYSTEM version 5.2

GES: CH-ST EL Y VA

ELEMENT VA SUSPENDED

SPECIES VA SUSPENDED

GES: L-ST

GAS CONSTANT IN USER ENERGY UNITS: 8.31451000E+00

1 BAR IN USER PRESSURE UNITS: 1.00000000E+05

CURRENT VALUE OF TEMPERATURE (KELVIN): 298.15

CURRENT VALUE OF PRESSURE (PASCAL): 1.00000000E+05

CURRENT NUMBER OF ELEMENT 4

ELEMENT	STABLE ELEMENT REFERENCE	MASS	H298-H0	S298
-1 /-	ELECTRON_GAS	0.0000E+00	0.0000E+00	0.0000E+00 E0000000
0 VA	VACUUM	0.0000E+00	0.0000E+00	0.0000E+00 E0000000
1 C	GRAPHITE	1.2011E+01	1.0540E+03	5.7400E+00 08000000
2 N	1/2 MOLE N2(GAS)	1.4007E+01	4.3350E+03	9.5751E+01 08000000
3 O	1/2 MOLE O2(GAS)	1.5999E+01	4.3410E+03	1.0252E+02 08000000
4 SI	DIAMOND_A4	2.8085E+01	3.2175E+03	1.8820E+01 08000000

CURRENT NUMBER OF PHASE 17

PHASE	STATUS	SUBLATTICES
1 GAS	88200000	1
2 BETA_QUARTZ	82200000	1
3 C1SI1_ALPHA	82200000	1
4 C1SI1_BETA	82200000	1
5 CRISTOBALITE	82200000	1
6 DIAMOND	82200000	1
7 GRAPHITE	82200000	1
8 GRAPHITE_L	82200000	1
9 N4SI3_S	82200000	1
10 QUARTZ	82200000	1
11 QUARTZ_S2	82200000	1
12 SiO2_LIQUID	82200000	1
13 SI_L	82200000	1
14 SI_S	82200000	1
15 TRIDYMIT	82200000	1
16 TRIDYMIT_S2	82200000	1
17 TRIDYMIT_S3	82200000	1

CURRENT NUMBER OF SPECIES 15

SPECIES	STOICHIOMETRY
1 C	80800000 C
2 C1O1	00000000 C1O1
3 C1O2	00000000 C1O2
4 C1SI1	00000000 C1SI1
5 C2	00000000 C2
6 C3	00000000 C3
7 N	80800000 N
8 N1O1	00000000 N1O1
9 N2	00000000 N2
10 N4SI3	00000000 N4SI3
11 O	80800000 O
12 O1SI1	00000000 O1SI1
13 O2	00000000 O2
14 O2SI1	00000000 O2SI1
15 SI	80800000 SI
16 VA	D1800000 VA

GES: GO R

Thermo-Calc REACTOR version 1.0

REACTOR: ?

AMEND_INPUT	CREATE_STAGE_BOXES	LIST_RECORDS
AMEND_RECORD	EQUILIBRATE	MACRO-FILE-OPEN
BACK	EXECUTE_POLY3_COMMAND	READ_WORKSPACE
CHANGE_SURROUNDINGS	EXIT	SAVE_WORKSPACE
CONTINUE_SIMULATION	GOTO_MODULE	SET_INTERACTIVE
CREATE_DIVIDERS	HELP	SHOW_PROBE
CREATE_PIPES	INFORMATION	START_SIMULATION
CREATE_PROBE	LIST_DESIGN	

```

REACTOR: @@ Create a reactor with 4 segments which is heat controlled.
REACTOR: @@ At the top segment 1 mole of quartz (SiO2) and 1.8 mole of graphite (C)
REACTOR: @@ is added. A small amount of N is also added to simplify calculations.
REACTOR: @@ The reactants have room temperature.
REACTOR: @@ In the other three segments only heat is added.
REACTOR: @@
REACTOR: @@ A guess of the initial temperature in each segment must be provided.
REACTOR: @@
REACTOR: CREATE_STAGE
NUMBER OF STAGE BOXES /4/: 4
YOU MUST FIRST DEFINE FEED FROM SURROUNDINGS!
GIVE FEED TO SYSTEM: N(C)=1.8
Input temperature /298.15/:
GIVE FEED TO SYSTEM: N(O2Si1)=1
Input temperature /298.15/:
GIVE FEED TO SYSTEM: H=876000
GIVE FEED TO SYSTEM: N(N2)=4e-4
Input temperature /298.15/:
GIVE FEED TO SYSTEM:

GIVE FOR STAGE BOX      1
NAME: /SEGMENT_1/:
TYPE OF BOX /EQUILIBRIUM/: EQUILIBRIUM
Is the stage heat controlled? /Y/: Y
Initial guess of temperature? /1000/: 1750
Give initial amount:
Each phase may have a separate output, give these
Phase name /REST/: gas
Phase name /REST/: REST

GIVE FOR STAGE BOX      2
NAME: /SEGMENT_2/:
TYPE OF BOX /EQUILIBRIUM/: EQUILIBRIUM
Is the stage heat controlled? /Y/: Y
Initial guess of temperature? /1000/: 1900
Give initial amount:
Each phase may have a separate output, give these
Phase name /REST/: gas
Phase name /REST/: REST

GIVE FOR STAGE BOX      3
NAME: /SEGMENT_3/:
TYPE OF BOX /EQUILIBRIUM/: EQUILIBRIUM
Is the stage heat controlled? /Y/: Y
Initial guess of temperature? /1000/: 2050
Give initial amount:
Each phase may have a separate output, give these
Phase name /REST/: gas
Phase name /REST/: REST

GIVE FOR STAGE BOX      4
NAME: /SEGMENT_4/:
TYPE OF BOX /EQUILIBRIUM/: EQUILIBRIUM
Is the stage heat controlled? /Y/: Y
Initial guess of temperature? /1000/: 2200
Give initial amount:
Each phase may have a separate output, give these
Phase name /REST/: gas
Phase name /REST/: REST
REACTOR: l-r

Number:  0 name: SURROUNDINGS           stage box at:   23,
Feed of C              with 1.8000E+00 mol to record:  -1
Feed of O2Si1          with 1.0000E+00 mol to record:  -1
Feed of heat 8.7600E+05 J to record:    -1
Feed of N2              with 4.0000E-04 mol to record:  -1

Number:  1 name: SEGMENT_1               stage box at:   72, H controlled
Output for phase GAS              to record:  -1
Output for phase REST              to record:  -1

Number:  2 name: SEGMENT_2               stage box at:  114, H controlled
Output for phase GAS              to record:  -1
Output for phase REST              to record:  -1

Number:  3 name: SEGMENT_3               stage box at:  156, H controlled
Output for phase GAS              to record:  -1
Output for phase REST              to record:  -1

Number:  4 name: SEGMENT_4               stage box at:  198, H controlled
Output for phase GAS              to record:  -1
Output for phase REST              to record:  -1
REACTOR: @@ Create dividers, one for distributing the gas from segment 2 to 4
REACTOR: @@ one for splitting the heat feed and one for splitting the feed on N2
REACTOR: create-div
Number of dividers /4/: 5
Number of outputs for divider 1: /3/: 2
Percent of input to output 1: /100/: 80
Number of outputs for divider 2: /3/: 3
Percent of input to output 1: /100/: 80 15
Number of outputs for divider 3: /3/: 3
Percent of input to output 1: /100/: 80 15
Number of outputs for divider 4: /3/: 3
Percent of input to output 1: /100/: 85 10
Number of outputs for divider 5: /3/: 4
Percent of input to output 1: /100/: 25 25 25
REACTOR: l-r

Number:  0 name: SURROUNDINGS           stage box at:   23,
Feed of C              with 1.8000E+00 mol to record:  -1
Feed of O2Si1          with 1.0000E+00 mol to record:  -1
Feed of heat 8.7600E+05 J to record:    -1
Feed of N2              with 4.0000E-04 mol to record:  -1

Number:  1 name: SEGMENT_1               stage box at:   72, H controlled
Output for phase GAS              to record:  -1
Output for phase REST              to record:  -1

Number:  2 name: SEGMENT_2               stage box at:  114, H controlled
Output for phase GAS              to record:  -1
Output for phase REST              to record:  -1

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```

Number: 3 name: SEGMENT_3                stage box at: 156, H controlled
Output for phase GAS                     to record: -1
Output for phase REST                     to record: -1

Number: 4 name: SEGMENT_4                stage box at: 198, H controlled
Output for phase GAS                     to record: -1
Output for phase REST                     to record: -1

Number: 5 name: DIVIDER_5                divider at: 240
80 % of input to record: -1
20 % of input to record: -1

Number: 6 name: DIVIDER_6                divider at: 268
80 % of input to record: -1
15 % of input to record: -1
5 % of input to record: -1

Number: 7 name: DIVIDER_7                divider at: 301
80 % of input to record: -1
15 % of input to record: -1
5 % of input to record: -1

Number: 8 name: DIVIDER_8                divider at: 334
85 % of input to record: -1
10 % of input to record: -1
5 % of input to record: -1

Number: 9 name: DIVIDER_9                divider at: 367
25 % of input to record: -1
25 % of input to record: -1
25 % of input to record: -1
25 % of input to record: -1
REACTOR: @@ Finally create the pipes between the segments first for the feed
REACTOR: c-pipe 0 1 1 8 9
Feed of C
Feed of O2SI1
Feed of heat
Input set to this divider
Feed of N2
Input set to this divider
NO MORE OUTPUT RECORDS
REACTOR: @@ All solid phases are assumed to go down one segment
REACTOR: @@ The gas phase is assumed to go up, 80% to the next segment,
REACTOR: @@ 15% to the second next and 5% to the third segment above.
REACTOR: @@ output from stage boxes
REACTOR: c-pipe 1 0 2
Output record for phase GAS
Output record for phase REST
NO MORE OUTPUT RECORDS
REACTOR: c-pipe 2 5 3
Output record for phase GAS
Input set to this divider
Output record for phase REST
NO MORE OUTPUT RECORDS
REACTOR: c-pipe 3 6 4
Output record for phase GAS
Input set to this divider
Output record for phase REST
NO MORE OUTPUT RECORDS
REACTOR: c-pipe 4 7 0
Output record for phase GAS
Input set to this divider
Output record for phase REST
NO MORE OUTPUT RECORDS
REACTOR: @@ output from dividers
REACTOR: c-pipe 5 1 0
Output record for 80 % of input
Output record for 20 % of input
NO MORE OUTPUT RECORDS
REACTOR: c-pipe 6 2 1 0
Output record for 80 % of input
Output record for 15 % of input
Output record for 5 % of input
NO MORE OUTPUT RECORDS
REACTOR: c-pipe 7 3 2 1
Output record for 80 % of input
Output record for 15 % of input
Output record for 5 % of input
NO MORE OUTPUT RECORDS
REACTOR: c-pipe 8 4 3 2
Output record for 85 % of input
Output record for 10 % of input
Output record for 5 % of input
NO MORE OUTPUT RECORDS
REACTOR: c-pipe 9 1 2 3 4
Output record for 25 % of input
Output record for 25 % of input
Output record for 25 % of input
Output record for 25 % of input
NO MORE OUTPUT RECORDS
REACTOR: 1-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 will consist of the conditions set in
REACTOR: @@ each segment, and the user may select some state variables also,
REACTOR: @@ in this case NP($ ) meaning moles of stable phases
REACTOR: @@ After each loop the temperatures in all segments are listed
REACTOR: @@
REACTOR: @@ We want to achive a reactor where only Si<L> leaves at the bottom.
REACTOR: START
Max number of loops: /10/: 50
OUTPUT TO SCREEN OR FILE /SCREEN/:
Output conditions? /Y/:
Output variables: /T BP($)/: T BP($ )
>>> DATA AT ITERATION 1 FROM STAGE 1
T=1750, P=1E5, N(C)=1.8, N(N)=2E-4, N(O)=2, N(SI)=1
DEGREES OF FREEDOM 0
T= 1.750000E+03
BP(GAS)=8.3899239E-3, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=3.9560636E-3, BP(CRISTOBALITE)=60.077021, BP(DIAMOND)=0,
BP(GRAPHITE)=21.616235, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 1 FROM STAGE 2
T=1900, P=1E5, N(C)=1.7998, N(N)=2E-4, N(O)=1.9998, N(SI)=0.999999
DEGREES OF FREEDOM 0
T= 1.900000E+03
BP(GAS)=35.781375, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=23.515817, BP(CRISTOBALITE)=22.402821, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 1 FROM STAGE 3
T=2050, P=1E5, N(C)=0.586488, N(N)=2E-4, N(O)=0.745729, N(SI)=0.959352
DEGREES OF FREEDOM 0
T= 2.050000E+03
BP(GAS)=1.1001909E-2, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=23.51327, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=22.396537, BP(SI_L)=6.3106228E-4,
BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 1 FROM STAGE 4
T=2200, P=1E5, N(C)=0.586424, N(N)=2E-4, N(O)=0.74552, N(SI)=0.959207
DEGREES OF FREEDOM 0
T= 2.200000E+03
BP(GAS)=27.369406, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=9.7781171, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=8.7657159, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 2 FROM STAGE 1
H=-9.69232E5, P=1E5, N(C)=2.78779, N(N)=4E-4, N(O)=3.04056, N(SI)=1.0527
DEGREES OF FREEDOM 0
T= 1.098651E+03
BP(GAS)=25.395955, BP(BETA_QUARTZ)=63.249404, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=0, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=23.055463, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 2 FROM STAGE 2
H=-8.37416E5, P=1E5, N(C)=1.97096, N(N)=3.9E-4, N(O)=2.2174, N(SI)=1.1133
DEGREES OF FREEDOM 0
T= 1.764644E+03
BP(GAS)=2.577188E-2, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=0.19891753, BP(CRISTOBALITE)=66.592185, BP(DIAMOND)=0,
BP(GRAPHITE)=23.605007, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 2 FROM STAGE 3
H=-7.72457E5, P=1E5, N(C)=2.24429, N(N)=3.6E-4, N(O)=2.81309, N(SI)=1.43588
DEGREES OF FREEDOM 0
T= 1.785830E+03
BP(GAS)=28.121362, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=21.054185, BP(CRISTOBALITE)=54.435284, BP(DIAMOND)=0,
BP(GRAPHITE)=8.6836041, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 2 FROM STAGE 4
H=33660.3, P=1E5, N(C)=1.24807, N(N)=2E-4, N(O)=1.812, N(SI)=1.4311
DEGREES OF FREEDOM 0
T= 2.447572E+03
BP(GAS)=60.210327, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=0.5584779, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=23.40707, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 3 FROM STAGE 1
H=-9.22751E5, P=1E5, N(C)=2.01172, N(N)=5.76E-4, N(O)=2.24134, N(SI)=1.02991
DEGREES OF FREEDOM 0

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```
T= 8.124883E+02
BP(GAS)=4.0693569, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0, BP(C1Si1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=23.005715,
BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=61.879868, BP(QUARTZ_S2)=0,
BP(SiO2_LIQUID)=0, BP(Si_L)=0, BP(Si_S)=0, BP(TRIDYMITE)=0,
BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION      3 FROM STAGE      2
H=-9.0397E5, P=1E5, N(C)=2.89749, N(N)=5.18E-4, N(O)=3.13248, N(Si)=1.12129
DEGREES OF FREEDOM 0
T= 1.746338E+03
BP(GAS)=25.042951, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0, BP(C1Si1_BETA)=0,
BP(CRISTOBALITE)=67.278274, BP(DIAMOND)=0, BP(GRAPHITE)=24.095798,
BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0,
BP(SiO2_LIQUID)=0, BP(Si_L)=0, BP(Si_S)=0, BP(TRIDYMITE)=0,
BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION      3 FROM STAGE      3
H=-8.04917E5, P=1E5, N(C)=2.99345, N(N)=3.6E-4, N(O)=3.68911, N(Si)=1.58674
DEGREES OF FREEDOM 0
T= 1.785838E+03
BP(GAS)=55.589669, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=28.960504, BP(CRISTOBALITE)=51.37138, BP(DIAMOND)=0,
BP(GRAPHITE)=3.6235819, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0, BP(Si_L)=0, BP(Si_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION      3 FROM STAGE      4
H=61307.1, P=1E5, N(C)=1.02397, N(N)=2E-4, N(O)=1.71001, N(Si)=1.57729
DEGREES OF FREEDOM 0
T= 2.594647E+03
BP(GAS)=59.391022, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0, BP(C1Si1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4Si3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0,
BP(Si_L)=24.567245, BP(Si_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION      4 FROM STAGE      1
H=-9.75673E5, P=1E5, N(C)=2.8597, N(N)=6.784E-4, N(O)=3.09674, N(Si)=1.03777
DEGREES OF FREEDOM 0
T= 1.067994E+03
BP(GAS)=27.303365, BP(BETA_QUARTZ)=62.352571, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=0, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=23.392027, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0, BP(Si_L)=0, BP(Si_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION      4 FROM STAGE      2
H=-9.26156E5, P=1E5, N(C)=3.67673, N(N)=5.18E-4, N(O)=3.91533, N(Si)=1.15072
DEGREES OF FREEDOM 0
T= 1.785833E+03
BP(GAS)=48.987037, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=2.2730168, BP(CRISTOBALITE)=65.232008, BP(DIAMOND)=0,
BP(GRAPHITE)=22.635726, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0, BP(Si_L)=0, BP(Si_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION      4 FROM STAGE      3
H=-7.59974E5, P=1E5, N(C)=2.76045, N(N)=3.6E-4, N(O)=3.53941, N(Si)=1.70442
DEGREES OF FREEDOM 0
T= 1.856422E+03
BP(GAS)=54.420155, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=34.739066, BP(CRISTOBALITE)=48.49715, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0, BP(Si_L)=0, BP(Si_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION      4 FROM STAGE      4
H=97718.1, P=1E5, N(C)=0.866397, N(N)=2E-4, N(O)=1.61434, N(Si)=1.67357
DEGREES OF FREEDOM 0
T= 2.773504E+03
BP(GAS)=58.669424, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0, BP(C1Si1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4Si3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0,
BP(Si_L)=24.569593, BP(Si_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION      5 FROM STAGE      1
H=-1.01358E6, P=1E5, N(C)=3.5158, N(N)=6.784E-4, N(O)=3.76462, N(Si)=1.05123
DEGREES OF FREEDOM 0
T= 1.163508E+03
BP(GAS)=45.980219, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0, BP(C1Si1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=22.850503,
BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0,
BP(SiO2_LIQUID)=0, BP(Si_L)=0, BP(Si_S)=0, BP(TRIDYMITE)=0,
BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=63.161004
>>> DATA AT ITERATION      5 FROM STAGE      2
H=-9.1327E5, P=1E5, N(C)=3.54766, N(N)=5.18E-4, N(O)=3.88466, N(Si)=1.19572
DEGREES OF FREEDOM 0
T= 1.785833E+03
BP(GAS)=49.603255, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=5.1279351, BP(CRISTOBALITE)=63.651652, BP(DIAMOND)=0,
BP(GRAPHITE)=19.968003, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0, BP(Si_L)=0, BP(Si_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION      5 FROM STAGE      3
H=-7.20023E5, P=1E5, N(C)=2.48349, N(N)=3.6E-4, N(O)=3.41026, N(Si)=1.82628
DEGREES OF FREEDOM 0
T= 1.974923E+03
BP(GAS)=54.111761, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=33.932787, BP(CRISTOBALITE)=47.641383, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0, BP(Si_L)=0, BP(Si_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION      5 FROM STAGE      4
H=1.21546E5, P=1E5, N(C)=0.846289, N(N)=2E-4, N(O)=1.58585, N(Si)=1.63921
DEGREES OF FREEDOM 0
T= 2.880121E+03
BP(GAS)=58.994116, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0, BP(C1Si1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4Si3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0,
BP(Si_L)=22.582856, BP(Si_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION      6 FROM STAGE      1
H=-1.01075E6, P=1E5, N(C)=3.49373, N(N)=6.784E-4, N(O)=3.76565,
N(Si)=1.07656
DEGREES OF FREEDOM 0
T= 1.245814E+03
BP(GAS)=44.984991, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0, BP(C1Si1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=22.786504,
BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0,
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      BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITE)=0,
      BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=64.683179
>>> DATA AT ITERATION      6 FROM STAGE      2
H=-9.07819E5, P=1E5, N(C)=3.33384, N(N)=5.18E-4, N(O)=3.85053, N(SI)=1.35148
DEGREES OF FREEDOM 0
T= 1.785834E+03
BP(GAS)=49.986926, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=12.328797, BP(CRISTOBALITE)=62.215897, BP(DIAMOND)=0,
BP(GRAPHITE)=15.079392, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION      6 FROM STAGE      3
H=-6.89982E5, P=1E5, N(C)=2.23998, N(N)=3.6E-4, N(O)=3.33968, N(SI)=2.01108
DEGREES OF FREEDOM 0
T= 2.024859E+03
BP(GAS)=55.901309, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=33.947223, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=46.973648, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION      6 FROM STAGE      4
H=1.42732E5, P=1E5, N(C)=0.846649, N(N)=2E-4, N(O)=1.56363, N(SI)=1.62846
DEGREES OF FREEDOM 0
T= 2.939413E+03
BP(GAS)=59.078725, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0, BP(C1S11_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
BP(SI_L)=21.844947, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION      7 FROM STAGE      1
H=-1.00894E6, P=1E5, N(C)=3.46804, N(N)=6.784E-4, N(O)=3.76822,
N(SI)=1.10673
DEGREES OF FREEDOM 0
T= 1.360090E+03
BP(GAS)=43.509998, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0, BP(C1S11_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=23.028873,
BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0,
BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITE)=0,
BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=66.495404
>>> DATA AT ITERATION      7 FROM STAGE      2
H=-9.0846E5, P=1E5, N(C)=3.15898, N(N)=5.18E-4, N(O)=3.86884, N(SI)=1.54042
DEGREES OF FREEDOM 0
T= 1.785834E+03
BP(GAS)=51.714964, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=20.759112, BP(CRISTOBALITE)=60.917489, BP(DIAMOND)=0,
BP(GRAPHITE)=9.7183695, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION      7 FROM STAGE      3
H=-6.68401E5, P=1E5, N(C)=2.00418, N(N)=3.6E-4, N(O)=3.27868, N(SI)=2.21214
DEGREES OF FREEDOM 0
T= 2.054719E+03
BP(GAS)=58.391066, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=34.178134, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=46.091552, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION      7 FROM STAGE      4
H=1.5752E5, P=1E5, N(C)=0.852408, N(N)=2E-4, N(O)=1.53426, N(SI)=1.61954
DEGREES OF FREEDOM 0
T= 2.970399E+03
BP(GAS)=58.350803, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0, BP(C1S11_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
BP(SI_L)=21.921684, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION      8 FROM STAGE      1
H=-1.01026E6, P=1E5, N(C)=3.48108, N(N)=6.784E-4, N(O)=3.81122,
N(SI)=1.13788
DEGREES OF FREEDOM 0
T= 1.482989E+03
BP(GAS)=43.00392, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0, BP(C1S11_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=23.382925,
BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0,
BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITE)=0,
BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=68.366928
>>> DATA AT ITERATION      8 FROM STAGE      2
H=-9.10878E5, P=1E5, N(C)=2.99607, N(N)=5.18E-4, N(O)=3.90142, N(SI)=1.7378
DEGREES OF FREEDOM 0
T= 1.785834E+03
BP(GAS)=53.79187, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=29.488666, BP(CRISTOBALITE)=59.674773, BP(DIAMOND)=0,
BP(GRAPHITE)=4.262819, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION      8 FROM STAGE      3
H=-6.55233E5, P=1E5, N(C)=1.77229, N(N)=3.6E-4, N(O)=3.21382, N(SI)=2.39985
DEGREES OF FREEDOM 0
T= 2.072919E+03
BP(GAS)=59.871555, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=34.480045, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=45.758102, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION      8 FROM STAGE      4
H=1.63921E5, P=1E5, N(C)=0.859937, N(N)=2E-4, N(O)=1.52316, N(SI)=1.62152
DEGREES OF FREEDOM 0
T= 2.980408E+03
BP(GAS)=57.971017, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0, BP(C1S11_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
BP(SI_L)=22.269931, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION      9 FROM STAGE      1
H=-1.01265E6, P=1E5, N(C)=3.50442, N(N)=6.784E-4, N(O)=3.86176, N(SI)=1.1655
DEGREES OF FREEDOM 0
T= 1.587698E+03
BP(GAS)=42.882393, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0, BP(C1S11_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=23.711015,
BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0,
BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITE)=0,
BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=70.024973
>>> DATA AT ITERATION      9 FROM STAGE      2

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H=-9.13276E5, P=1E5, N(C)=2.83298, N(N)=5.18E-4, N(O)=3.91194, N(SI)=1.91242
DEGREES OF FREEDOM 0
T= 1.813659E+03
BP(GAS)=54.528551, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=36.500134, BP(CRISTOBALITE)=59.303002, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0, BP(TRIDYMITTE_S3)=0
>>> DATA AT ITERATION 9 FROM STAGE 3
H=-6.54501E5, P=1E5, N(C)=1.59827, N(N)=3.6E-4, N(O)=3.19257, N(SI)=2.56019
DEGREES OF FREEDOM 0
T= 2.082775E+03
BP(GAS)=61.270691, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=34.761699, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=46.15036, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0, BP(TRIDYMITTE_S3)=0
>>> DATA AT ITERATION 9 FROM STAGE 4
H=1.60038E5, P=1E5, N(C)=0.866962, N(N)=2E-4, N(O)=1.53622, N(SI)=1.63507
DEGREES OF FREEDOM 0
T= 2.968716E+03
BP(GAS)=58.165846, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
BP(SI_L)=22.749015, BP(SI_S)=0, BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0,
BP(TRIDYMITTE_S3)=0
=====
>>> DATA AT ITERATION 10 FROM STAGE 1
H=-1.01175E6, P=1E5, N(C)=3.49117, N(N)=6.784E-4, N(O)=3.87559,
N(SI)=1.19209
DEGREES OF FREEDOM 0
T= 1.688378E+03
BP(GAS)=41.818997, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=24.015589,
BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0,
BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITTE)=0,
BP(TRIDYMITTE_S2)=0, BP(TRIDYMITTE_S3)=71.592751
>>> DATA AT ITERATION 10 FROM STAGE 2
H=-9.17571E5, P=1E5, N(C)=2.71456, N(N)=5.18E-4, N(O)=3.93864, N(SI)=2.05542
DEGREES OF FREEDOM 0
T= 1.931654E+03
BP(GAS)=54.443868, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=37.245343, BP(CRISTOBALITE)=61.663362, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0, BP(TRIDYMITTE_S3)=0
>>> DATA AT ITERATION 10 FROM STAGE 3
H=-6.75806E5, P=1E5, N(C)=1.62247, N(N)=3.6E-4, N(O)=3.28158, N(SI)=2.61526
DEGREES OF FREEDOM 0
T= 2.082796E+03
BP(GAS)=62.678063, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=35.079061, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=47.68706, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0, BP(TRIDYMITTE_S3)=0
>>> DATA AT ITERATION 10 FROM STAGE 4
H=1.40325E5, P=1E5, N(C)=0.874877, N(N)=2E-4, N(O)=1.58737, N(SI)=1.66856
DEGREES OF FREEDOM 0
T= 2.917962E+03
BP(GAS)=59.278419, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
BP(SI_L)=23.490504, BP(SI_S)=0, BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0,
BP(TRIDYMITTE_S3)=0
=====
>>> DATA AT ITERATION 11 FROM STAGE 1
H=-1.00311E6, P=1E5, N(C)=3.3844, N(N)=6.784E-4, N(O)=3.84233, N(SI)=1.26378
DEGREES OF FREEDOM 0
T= 1.785825E+03
BP(GAS)=40.181412, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=2.0429794, BP(CRISTOBALITE)=72.460051, BP(DIAMOND)=0,
BP(GRAPHITE)=22.941883, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0, BP(TRIDYMITTE_S3)=0
>>> DATA AT ITERATION 11 FROM STAGE 2
H=-9.22617E5, P=1E5, N(C)=2.69033, N(N)=5.18E-4, N(O)=4.00547, N(SI)=2.13913
DEGREES OF FREEDOM 0
T= 1.964263E+03
BP(GAS)=56.690324, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=37.355782, BP(CRISTOBALITE)=62.435822, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0, BP(TRIDYMITTE_S3)=0
>>> DATA AT ITERATION 11 FROM STAGE 3
H=-6.99253E5, P=1E5, N(C)=1.63156, N(N)=3.6E-4, N(O)=3.34822, N(SI)=2.63654
DEGREES OF FREEDOM 0
T= 2.082357E+03
BP(GAS)=62.812321, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=34.943937, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=49.460883, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0, BP(TRIDYMITTE_S3)=0
>>> DATA AT ITERATION 11 FROM STAGE 4
H=1.17365E5, P=1E5, N(C)=0.871507, N(N)=2E-4, N(O)=1.64642, N(SI)=1.69472
DEGREES OF FREEDOM 0
T= 2.855981E+03
BP(GAS)=60.986549, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
BP(SI_L)=23.421073, BP(SI_S)=0, BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0,
BP(TRIDYMITTE_S3)=0
=====
>>> DATA AT ITERATION 12 FROM STAGE 1
H=-1.00345E6, P=1E5, N(C)=3.36452, N(N)=6.784E-4, N(O)=3.87931,
N(SI)=1.31896
DEGREES OF FREEDOM 0
T= 1.785826E+03
BP(GAS)=41.745842, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=4.6200248, BP(CRISTOBALITE)=71.897832, BP(DIAMOND)=0,
BP(GRAPHITE)=21.265337, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0, BP(TRIDYMITTE_S3)=0
>>> DATA AT ITERATION 12 FROM STAGE 2
H=-9.23112E5, P=1E5, N(C)=2.62448, N(N)=5.18E-4, N(O)=4.00169, N(SI)=2.19444
DEGREES OF FREEDOM 0
T= 1.981583E+03

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BP(GAS)=56.956864, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=37.363041, BP(CRISTOBALITE)=62.863929, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0, BP(Si_L)=0, BP(Si_S)=0,
BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0, BP(TRIDYMITTE_S3)=0
>>> DATA AT ITERATION 12 FROM STAGE 3
H=-7.19679E5, P=1E5, N(C)=1.62905, N(N)=3.6E-4, N(O)=3.4097, N(SI)=2.66675
DEGREES OF FREEDOM 0
T= 2.082497E+03
BP(GAS)=63.219192, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=34.784904, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=51.014914, BP(Si_L)=0, BP(Si_S)=0,
BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0, BP(TRIDYMITTE_S3)=0
>>> DATA AT ITERATION 12 FROM STAGE 4
H=97299.2, P=1E5, N(C)=0.867541, N(N)=2E-4, N(O)=1.69815, N(SI)=1.71661
DEGREES OF FREEDOM 0
T= 2.791245E+03
BP(GAS)=62.594968, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0, BP(C1Si1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4Si3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0,
BP(Si_L)=23.207652, BP(Si_S)=0, BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0,
BP(TRIDYMITTE_S3)=0
=====
>>> DATA AT ITERATION 13 FROM STAGE 1
H=-1.00205E6, P=1E5, N(C)=3.31172, N(N)=6.784E-4, N(O)=3.86893,
N(SI)=1.36009
DEGREES OF FREEDOM 0
T= 1.785826E+03
BP(GAS)=41.7826, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=6.5030761, BP(CRISTOBALITE)=71.546701, BP(DIAMOND)=0,
BP(GRAPHITE)=20.051342, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0, BP(Si_L)=0, BP(Si_S)=0,
BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0, BP(TRIDYMITTE_S3)=0
>>> DATA AT ITERATION 13 FROM STAGE 2
H=-9.24576E5, P=1E5, N(C)=2.57094, N(N)=5.18E-4, N(O)=4.00556, N(SI)=2.24663
DEGREES OF FREEDOM 0
T= 1.994519E+03
BP(GAS)=57.417428, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=37.390387, BP(CRISTOBALITE)=63.260705, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0, BP(Si_L)=0, BP(Si_S)=0,
BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0, BP(TRIDYMITTE_S3)=0
>>> DATA AT ITERATION 13 FROM STAGE 3
H=-7.374E5, P=1E5, N(C)=1.62655, N(N)=3.6E-4, N(O)=3.4643, N(SI)=2.69763
DEGREES OF FREEDOM 0
T= 2.082731E+03
BP(GAS)=63.654312, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=34.710227, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=52.365328, BP(Si_L)=0, BP(Si_S)=0,
BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0, BP(TRIDYMITTE_S3)=0
>>> DATA AT ITERATION 13 FROM STAGE 4
H=79895.2, P=1E5, N(C)=0.865678, N(N)=2E-4, N(O)=1.7431, N(SI)=1.73723
DEGREES OF FREEDOM 0
T= 2.721648E+03
BP(GAS)=64.038962, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0, BP(C1Si1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4Si3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0,
BP(Si_L)=23.039395, BP(Si_S)=0, BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0,
BP(TRIDYMITTE_S3)=0
=====
>>> DATA AT ITERATION 14 FROM STAGE 1
H=-1.00119E6, P=1E5, N(C)=3.26815, N(N)=6.784E-4, N(O)=3.86516,
N(SI)=1.39888
DEGREES OF FREEDOM 0
T= 1.785826E+03
BP(GAS)=41.977202, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=8.2717561, BP(CRISTOBALITE)=71.225272, BP(DIAMOND)=0,
BP(GRAPHITE)=18.915409, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0, BP(Si_L)=0, BP(Si_S)=0,
BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0, BP(TRIDYMITTE_S3)=0
>>> DATA AT ITERATION 14 FROM STAGE 2
H=-9.25814E5, P=1E5, N(C)=2.51969, N(N)=5.18E-4, N(O)=4.00932, N(SI)=2.2976
DEGREES OF FREEDOM 0
T= 2.001975E+03
BP(GAS)=56.899727, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=37.678344, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=64.366461, BP(Si_L)=0, BP(Si_S)=0,
BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0, BP(TRIDYMITTE_S3)=0
>>> DATA AT ITERATION 14 FROM STAGE 3
H=-7.5344E5, P=1E5, N(C)=1.63225, N(N)=3.6E-4, N(O)=3.53706, N(SI)=2.7445
DEGREES OF FREEDOM 0
T= 2.083146E+03
BP(GAS)=65.078538, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=34.68776, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=53.512479, BP(Si_L)=0, BP(Si_S)=0,
BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0, BP(TRIDYMITTE_S3)=0
>>> DATA AT ITERATION 14 FROM STAGE 4
H=65149.9, P=1E5, N(C)=0.865118, N(N)=2E-4, N(O)=1.78129, N(SI)=1.75576
DEGREES OF FREEDOM 0
T= 2.649675E+03
BP(GAS)=65.327667, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0, BP(C1Si1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4Si3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0,
BP(Si_L)=22.875373, BP(Si_S)=0, BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0,
BP(TRIDYMITTE_S3)=0
=====
>>> DATA AT ITERATION 15 FROM STAGE 1
H=-9.99863E5, P=1E5, N(C)=3.22232, N(N)=6.784E-4, N(O)=3.84582,
N(SI)=1.42466
DEGREES OF FREEDOM 0
T= 1.785826E+03
BP(GAS)=41.607103, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=9.4314288, BP(CRISTOBALITE)=71.039976, BP(DIAMOND)=0,
BP(GRAPHITE)=18.175039, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0, BP(Si_L)=0, BP(Si_S)=0,
BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0, BP(TRIDYMITTE_S3)=0
>>> DATA AT ITERATION 15 FROM STAGE 2
H=-9.28208E5, P=1E5, N(C)=2.49189, N(N)=5.18E-4, N(O)=4.03654, N(SI)=2.34977
DEGREES OF FREEDOM 0
T= 2.011374E+03
BP(GAS)=58.095641, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=37.727938, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,

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BP (GRAPHITE)=0, BP (GRAPHITE_L)=0, BP (N4SI3_S)=0, BP (QUARTZ)=0,
BP (QUARTZ_S2)=0, BP (SIO2_LIQUID)=64.687647, BP (SI_L)=0, BP (SI_S)=0,
BP (TRIDYMITE)=0, BP (TRIDYMITE_S2)=0, BP (TRIDYMITE_S3)=0
>>> DATA AT ITERATION 15 FROM STAGE 3
H=-7.66271E5, P=1E5, N(C)=1.63303, N(N)=3.6E-4, N(O)=3.5783, N(SI)=2.77058
DEGREES OF FREEDOM 0
T= 2.083324E+03
BP (GAS)=65.468307, BP (BETA_QUARTZ)=0, BP (C1SI1_ALPHA)=0,
BP (C1SI1_BETA)=34.724895, BP (CRISTOBALITE)=0, BP (DIAMOND)=0,
BP (GRAPHITE)=0, BP (GRAPHITE_L)=0, BP (N4SI3_S)=0, BP (QUARTZ)=0,
BP (QUARTZ_S2)=0, BP (SIO2_LIQUID)=54.487318, BP (SI_L)=0, BP (SI_S)=0,
BP (TRIDYMITE)=0, BP (TRIDYMITE_S2)=0, BP (TRIDYMITE_S3)=0
>>> DATA AT ITERATION 15 FROM STAGE 4
H=52616., P=1E5, N(C)=0.866044, N(N)=2E-4, N(O)=1.81373, N(SI)=1.77291
DEGREES OF FREEDOM 0
T= 2.575865E+03
BP (GAS)=66.4689, BP (BETA_QUARTZ)=0, BP (C1SI1_ALPHA)=0, BP (C1SI1_BETA)=0,
BP (CRISTOBALITE)=0, BP (DIAMOND)=0, BP (GRAPHITE)=0, BP (GRAPHITE_L)=0,
BP (N4SI3_S)=0, BP (QUARTZ)=0, BP (QUARTZ_S2)=0, BP (SIO2_LIQUID)=0,
BP (SI_L)=22.746115, BP (SI_S)=0, BP (TRIDYMITE)=0, BP (TRIDYMITE_S2)=0,
BP (TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 16 FROM STAGE 1
H=-1.00007E6, P=1E5, N(C)=3.19911, N(N)=6.784E-4, N(O)=3.86199,
N(SI)=1.46355
DEGREES OF FREEDOM 0
T= 1.785826E+03
BP (GAS)=42.375412, BP (BETA_QUARTZ)=0, BP (C1SI1_ALPHA)=0,
BP (C1SI1_BETA)=11.209868, BP (CRISTOBALITE)=70.703913, BP (DIAMOND)=0,
BP (GRAPHITE)=17.036612, BP (GRAPHITE_L)=0, BP (N4SI3_S)=0, BP (QUARTZ)=0,
BP (QUARTZ_S2)=0, BP (SIO2_LIQUID)=0, BP (SI_L)=0, BP (SI_S)=0,
BP (TRIDYMITE)=0, BP (TRIDYMITE_S2)=0, BP (TRIDYMITE_S3)=0
>>> DATA AT ITERATION 16 FROM STAGE 2
H=-9.28527E5, P=1E5, N(C)=2.44149, N(N)=5.18E-4, N(O)=4.03726, N(SI)=2.39893
DEGREES OF FREEDOM 0
T= 2.020037E+03
BP (GAS)=58.591619, BP (BETA_QUARTZ)=0, BP (C1SI1_ALPHA)=0,
BP (C1SI1_BETA)=37.771357, BP (CRISTOBALITE)=0, BP (DIAMOND)=0,
BP (GRAPHITE)=0, BP (GRAPHITE_L)=0, BP (N4SI3_S)=0, BP (QUARTZ)=0,
BP (QUARTZ_S2)=0, BP (SIO2_LIQUID)=64.935199, BP (SI_L)=0, BP (SI_S)=0,
BP (TRIDYMITE)=0, BP (TRIDYMITE_S2)=0, BP (TRIDYMITE_S3)=0
>>> DATA AT ITERATION 16 FROM STAGE 3
H=-7.76568E5, P=1E5, N(C)=1.63486, N(N)=3.6E-4, N(O)=3.6125, N(SI)=2.79319
DEGREES OF FREEDOM 0
T= 2.083472E+03
BP (GAS)=65.828608, BP (BETA_QUARTZ)=0, BP (C1SI1_ALPHA)=0,
BP (C1SI1_BETA)=34.789071, BP (CRISTOBALITE)=0, BP (DIAMOND)=0,
BP (GRAPHITE)=0, BP (GRAPHITE_L)=0, BP (N4SI3_S)=0, BP (QUARTZ)=0,
BP (QUARTZ_S2)=0, BP (SIO2_LIQUID)=55.266798, BP (SI_L)=0, BP (SI_S)=0,
BP (TRIDYMITE)=0, BP (TRIDYMITE_S2)=0, BP (TRIDYMITE_S3)=0
>>> DATA AT ITERATION 16 FROM STAGE 4
H=42605.4, P=1E5, N(C)=0.867644, N(N)=2E-4, N(O)=1.83968, N(SI)=1.78749
DEGREES OF FREEDOM 0
T= 2.507707E+03
BP (GAS)=67.422071, BP (BETA_QUARTZ)=0, BP (C1SI1_ALPHA)=0, BP (C1SI1_BETA)=0,
BP (CRISTOBALITE)=0, BP (DIAMOND)=0, BP (GRAPHITE)=0, BP (GRAPHITE_L)=0,
BP (N4SI3_S)=0, BP (QUARTZ)=0, BP (QUARTZ_S2)=0, BP (SIO2_LIQUID)=0,
BP (SI_L)=22.6366, BP (SI_S)=0, BP (TRIDYMITE)=0, BP (TRIDYMITE_S2)=0,
BP (TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 17 FROM STAGE 1
H=-9.99181E5, P=1E5, N(C)=3.15804, N(N)=6.784E-4, N(O)=3.8585, N(SI)=1.50085
DEGREES OF FREEDOM 0
T= 1.785826E+03
BP (GAS)=42.570553, BP (BETA_QUARTZ)=0, BP (C1SI1_ALPHA)=0,
BP (C1SI1_BETA)=12.913325, BP (CRISTOBALITE)=70.390441, BP (DIAMOND)=0,
BP (GRAPHITE)=15.949972, BP (GRAPHITE_L)=0, BP (N4SI3_S)=0, BP (QUARTZ)=0,
BP (QUARTZ_S2)=0, BP (SIO2_LIQUID)=0, BP (SI_L)=0, BP (SI_S)=0,
BP (TRIDYMITE)=0, BP (TRIDYMITE_S2)=0, BP (TRIDYMITE_S3)=0
>>> DATA AT ITERATION 17 FROM STAGE 2
H=-9.28656E5, P=1E5, N(C)=2.39392, N(N)=5.18E-4, N(O)=4.03732, N(SI)=2.4454
DEGREES OF FREEDOM 0
T= 2.027376E+03
BP (GAS)=59.074267, BP (BETA_QUARTZ)=0, BP (C1SI1_ALPHA)=0,
BP (C1SI1_BETA)=37.816728, BP (CRISTOBALITE)=0, BP (DIAMOND)=0,
BP (GRAPHITE)=0, BP (GRAPHITE_L)=0, BP (N4SI3_S)=0, BP (QUARTZ)=0,
BP (QUARTZ_S2)=0, BP (SIO2_LIQUID)=65.141742, BP (SI_L)=0, BP (SI_S)=0,
BP (TRIDYMITE)=0, BP (TRIDYMITE_S2)=0, BP (TRIDYMITE_S3)=0
>>> DATA AT ITERATION 17 FROM STAGE 3
H=-7.84668E5, P=1E5, N(C)=1.63727, N(N)=3.6E-4, N(O)=3.64014, N(SI)=2.81254
DEGREES OF FREEDOM 0
T= 2.083598E+03
BP (GAS)=66.144587, BP (BETA_QUARTZ)=0, BP (C1SI1_ALPHA)=0,
BP (C1SI1_BETA)=34.875517, BP (CRISTOBALITE)=0, BP (DIAMOND)=0,
BP (GRAPHITE)=0, BP (GRAPHITE_L)=0, BP (N4SI3_S)=0, BP (QUARTZ)=0,
BP (QUARTZ_S2)=0, BP (SIO2_LIQUID)=55.878823, BP (SI_L)=0, BP (SI_S)=0,
BP (TRIDYMITE)=0, BP (TRIDYMITE_S2)=0, BP (TRIDYMITE_S3)=0
>>> DATA AT ITERATION 17 FROM STAGE 4
H=34757.6, P=1E5, N(C)=0.8698, N(N)=2E-4, N(O)=1.86005, N(SI)=1.79983
DEGREES OF FREEDOM 0
T= 2.447966E+03
BP (GAS)=68.189731, BP (BETA_QUARTZ)=0, BP (C1SI1_ALPHA)=0, BP (C1SI1_BETA)=0,
BP (CRISTOBALITE)=0, BP (DIAMOND)=0, BP (GRAPHITE)=0, BP (GRAPHITE_L)=0,
BP (N4SI3_S)=0, BP (QUARTZ)=0, BP (QUARTZ_S2)=0, BP (SIO2_LIQUID)=0,
BP (SI_L)=22.567411, BP (SI_S)=0, BP (TRIDYMITE)=0, BP (TRIDYMITE_S2)=0,
BP (TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 18 FROM STAGE 1
H=-9.98331E5, P=1E5, N(C)=3.11923, N(N)=6.784E-4, N(O)=3.85516,
N(SI)=1.53616
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP (GAS)=42.754622, BP (BETA_QUARTZ)=0, BP (C1SI1_ALPHA)=0,
BP (C1SI1_BETA)=14.526169, BP (CRISTOBALITE)=70.09308, BP (DIAMOND)=0,
BP (GRAPHITE)=14.922319, BP (GRAPHITE_L)=0, BP (N4SI3_S)=0, BP (QUARTZ)=0,
BP (QUARTZ_S2)=0, BP (SIO2_LIQUID)=0, BP (SI_L)=0, BP (SI_S)=0,
BP (TRIDYMITE)=0, BP (TRIDYMITE_S2)=0, BP (TRIDYMITE_S3)=0
>>> DATA AT ITERATION 18 FROM STAGE 2
H=-9.28547E5, P=1E5, N(C)=2.34912, N(N)=5.18E-4, N(O)=4.03628, N(SI)=2.4885
DEGREES OF FREEDOM 0
T= 2.033605E+03
BP (GAS)=59.522046, BP (BETA_QUARTZ)=0, BP (C1SI1_ALPHA)=0,
BP (C1SI1_BETA)=37.858508, BP (CRISTOBALITE)=0, BP (DIAMOND)=0,
BP (GRAPHITE)=0, BP (GRAPHITE_L)=0, BP (N4SI3_S)=0, BP (QUARTZ)=0,
BP (QUARTZ_S2)=0, BP (SIO2_LIQUID)=65.307945, BP (SI_L)=0, BP (SI_S)=0,
BP (TRIDYMITE)=0, BP (TRIDYMITE_S2)=0, BP (TRIDYMITE_S3)=0

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>>> DATA AT ITERATION 18 FROM STAGE 3
H=-7.9095E5, P=1E5, N(C)=1.64004, N(N)=3.6E-4, N(O)=3.66197, N(SI)=2.82819
DEGREES OF FREEDOM 0
T= 2.083688E+03
BP(GAS)=66.403735, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=34.965075, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=56.352228, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 18 FROM STAGE 4
H=28693.4, P=1E5, N(C)=0.872034, N(N)=2E-4, N(O)=1.87581, N(SI)=1.80994
DEGREES OF FREEDOM 0
T= 2.398232E+03
BP(GAS)=68.793565, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
BP(SI_L)=22.52654, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 19 FROM STAGE 1
H=-9.97507E5, P=1E5, N(C)=3.08274, N(N)=6.784E-4, N(O)=3.8516, N(SI)=1.569
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=42.913713, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=16.0268, BP(CRISTOBALITE)=69.816122, BP(DIAMOND)=0,
BP(GRAPHITE)=13.966842, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 19 FROM STAGE 2
H=-9.28273E5, P=1E5, N(C)=2.30776, N(N)=5.18E-4, N(O)=4.03429, N(SI)=2.52748
DEGREES OF FREEDOM 0
T= 2.038832E+03
BP(GAS)=59.919125, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=37.894909, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.440555, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 19 FROM STAGE 3
H=-7.95775E5, P=1E5, N(C)=1.64273, N(N)=3.6E-4, N(O)=3.67899, N(SI)=2.84056
DEGREES OF FREEDOM 0
T= 2.083751E+03
BP(GAS)=66.611155, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=35.046897, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=56.715065, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 19 FROM STAGE 4
H=24048.8, P=1E5, N(C)=0.874075, N(N)=2E-4, N(O)=1.88789, N(SI)=1.81802
DEGREES OF FREEDOM 0
T= 2.358285E+03
BP(GAS)=69.261131, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
BP(SI_L)=22.503633, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 20 FROM STAGE 1
H=-9.96727E5, P=1E5, N(C)=3.04912, N(N)=6.784E-4, N(O)=3.84782,
N(SI)=1.59879
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.042147, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=17.387655, BP(CRISTOBALITE)=69.565062, BP(DIAMOND)=0,
BP(GRAPHITE)=13.100767, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 20 FROM STAGE 2
H=-9.27909E5, P=1E5, N(C)=2.27042, N(N)=5.18E-4, N(O)=4.03169, N(SI)=2.56201
DEGREES OF FREEDOM 0
T= 2.043175E+03
BP(GAS)=60.26286, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=37.925513, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.546005, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 20 FROM STAGE 3
H=-7.99465E5, P=1E5, N(C)=1.64513, N(N)=3.6E-4, N(O)=3.69216, N(SI)=2.85019
DEGREES OF FREEDOM 0
T= 2.083795E+03
BP(GAS)=66.774912, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=35.116372, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=56.991941, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 20 FROM STAGE 4
H=20506.2, P=1E5, N(C)=0.875807, N(N)=2E-4, N(O)=1.89711, N(SI)=1.82436
DEGREES OF FREEDOM 0
T= 2.326902E+03
BP(GAS)=69.620213, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
BP(SI_L)=22.490901, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 21 FROM STAGE 1
H=-9.96006E5, P=1E5, N(C)=3.01883, N(N)=6.784E-4, N(O)=3.84399,
N(SI)=1.62523
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.142842, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=18.595742, BP(CRISTOBALITE)=69.342396, BP(DIAMOND)=0,
BP(GRAPHITE)=12.332156, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 21 FROM STAGE 2
H=-9.27508E5, P=1E5, N(C)=2.23735, N(N)=5.18E-4, N(O)=4.02883, N(SI)=2.59209
DEGREES OF FREEDOM 0
T= 2.046761E+03
BP(GAS)=60.555657, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=37.95068, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.629721, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 21 FROM STAGE 3
H=-8.02281E5, P=1E5, N(C)=1.64714, N(N)=3.6E-4, N(O)=3.70232, N(SI)=2.85765
DEGREES OF FREEDOM 0

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T= 2.083827E+03
BP(GAS)=66.903686, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=35.172894, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=57.202793, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 21 FROM STAGE 4
H=17809.2, P=1E5, N(C)=0.877217, N(N)=2E-4, N(O)=1.90413, N(SI)=1.82928
DEGREES OF FREEDOM 0
T= 2.302569E+03
BP(GAS)=69.894815, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0, BP(C1Si1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4Si3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0,
BP(SI_L)=22.483673, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 22 FROM STAGE 1
H=-9.95358E5, P=1E5, N(C)=2.99203, N(N)=6.784E-4, N(O)=3.84029,
N(SI)=1.64831
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.220494, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=19.650414, BP(CRISTOBALITE)=69.148215, BP(DIAMOND)=0,
BP(GRAPHITE)=11.661297, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 22 FROM STAGE 2
H=-9.27105E5, P=1E5, N(C)=2.20849, N(N)=5.18E-4, N(O)=4.02593, N(SI)=2.61797
DEGREES OF FREEDOM 0
T= 2.049708E+03
BP(GAS)=60.802621, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=37.971114, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=65.696163, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 22 FROM STAGE 3
H=-8.04427E5, P=1E5, N(C)=1.64878, N(N)=3.6E-4, N(O)=3.71015, N(SI)=2.86341
DEGREES OF FREEDOM 0
T= 2.083850E+03
BP(GAS)=67.004966, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=35.217743, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=57.363223, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 22 FROM STAGE 4
H=15757.7, P=1E5, N(C)=0.878336, N(N)=2E-4, N(O)=1.90947, N(SI)=1.83307
DEGREES OF FREEDOM 0
T= 2.283845E+03
BP(GAS)=70.104344, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0, BP(C1Si1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4Si3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0,
BP(SI_L)=22.479422, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 23 FROM STAGE 1
H=-9.94784E5, P=1E5, N(C)=2.96867, N(N)=6.784E-4, N(O)=3.83684,
N(SI)=1.66821
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.280013, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=20.559619, BP(CRISTOBALITE)=68.980974, BP(DIAMOND)=0,
BP(GRAPHITE)=11.083055, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 23 FROM STAGE 2
H=-9.26721E5, P=1E5, N(C)=2.18361, N(N)=5.18E-4, N(O)=4.02315, N(SI)=2.64002
DEGREES OF FREEDOM 0
T= 2.052127E+03
BP(GAS)=61.009565, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=37.987587, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=65.748921, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 23 FROM STAGE 3
H=-8.06062E5, P=1E5, N(C)=1.65008, N(N)=3.6E-4, N(O)=3.71618, N(SI)=2.86785
DEGREES OF FREEDOM 0
T= 2.083867E+03
BP(GAS)=67.084737, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=35.252804, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=57.485245, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 23 FROM STAGE 4
H=14197.5, P=1E5, N(C)=0.87921, N(N)=2E-4, N(O)=1.91353, N(SI)=1.83597
DEGREES OF FREEDOM 0
T= 2.269500E+03
BP(GAS)=70.264028, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0, BP(C1Si1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4Si3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0,
BP(SI_L)=22.476822, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 24 FROM STAGE 1
H=-9.94284E5, P=1E5, N(C)=2.94854, N(N)=6.784E-4, N(O)=3.83371,
N(SI)=1.68521
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.325561, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=21.335974, BP(CRISTOBALITE)=68.838274, BP(DIAMOND)=0,
BP(GRAPHITE)=10.589356, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 24 FROM STAGE 2
H=-9.26367E5, P=1E5, N(C)=2.16234, N(N)=5.18E-4, N(O)=4.02059, N(SI)=2.65869
DEGREES OF FREEDOM 0
T= 2.054109E+03
BP(GAS)=61.182133, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=38.000817, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=65.790849, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 24 FROM STAGE 3
H=-8.07308E5, P=1E5, N(C)=1.65111, N(N)=3.6E-4, N(O)=3.72082, N(SI)=2.87127
DEGREES OF FREEDOM 0
T= 2.083880E+03
BP(GAS)=67.147679, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
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BP(C1S11_BETA)=35.279965, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.578045, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 24 FROM STAGE 4
H=13011.1, P=1E5, N(C)=0.879887, N(N)=2E-4, N(O)=1.91662, N(SI)=1.8382
DEGREES OF FREEDOM 0
T= 2.258539E+03
BP(GAS)=70.385643, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0, BP(C1S11_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
BP(SI_L)=22.475169, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 25 FROM STAGE 1
H=-9.93853E5, P=1E5, N(C)=2.93135, N(N)=6.784E-4, N(O)=3.83093,
N(SI)=1.69961
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.360421, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=21.993986, BP(CRISTOBALITE)=68.717389, BP(DIAMOND)=0,
BP(GRAPHITE)=10.170946, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 25 FROM STAGE 2
H=-9.26049E5, P=1E5, N(C)=2.1443, N(N)=5.18E-4, N(O)=4.01827, N(SI)=2.67439
DEGREES OF FREEDOM 0
T= 2.055734E+03
BP(GAS)=61.325484, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=38.011422, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.824207, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 25 FROM STAGE 3
H=-8.08257E5, P=1E5, N(C)=1.65192, N(N)=3.6E-4, N(O)=3.7244, N(SI)=2.87392
DEGREES OF FREEDOM 0
T= 2.083891E+03
BP(GAS)=67.197432, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=35.300889, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.648624, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 25 FROM STAGE 4
H=12109., P=1E5, N(C)=0.880409, N(N)=2E-4, N(O)=1.91897, N(SI)=1.83989
DEGREES OF FREEDOM 0
T= 2.250176E+03
BP(GAS)=70.47823, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0, BP(C1S11_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
BP(SI_L)=22.474083, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 26 FROM STAGE 1
H=-9.93484E5, P=1E5, N(C)=2.91678, N(N)=6.784E-4, N(O)=3.82849,
N(SI)=1.71175
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.387119, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=22.548384, BP(CRISTOBALITE)=68.615573, BP(DIAMOND)=0,
BP(GRAPHITE)=9.8184387, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 26 FROM STAGE 2
H=-9.25767E5, P=1E5, N(C)=2.12908, N(N)=5.18E-4, N(O)=4.01622, N(SI)=2.68754
DEGREES OF FREEDOM 0
T= 2.057064E+03
BP(GAS)=61.444184, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=38.019917, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.850777, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 26 FROM STAGE 3
H=-8.08981E5, P=1E5, N(C)=1.65255, N(N)=3.6E-4, N(O)=3.72717, N(SI)=2.87596
DEGREES OF FREEDOM 0
T= 2.083898E+03
BP(GAS)=67.236826, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=35.316945, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.702307, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 26 FROM STAGE 4
H=11422.8, P=1E5, N(C)=0.88081, N(N)=2E-4, N(O)=1.92075, N(SI)=1.84119
DEGREES OF FREEDOM 0
T= 2.243802E+03
BP(GAS)=70.548706, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0, BP(C1S11_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
BP(SI_L)=22.473348, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 27 FROM STAGE 1
H=-9.93171E5, P=1E5, N(C)=2.90449, N(N)=6.784E-4, N(O)=3.82638,
N(SI)=1.72193
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.407584, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=23.013201, BP(CRISTOBALITE)=68.530223, BP(DIAMOND)=0,
BP(GRAPHITE)=9.5229002, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 27 FROM STAGE 2
H=-9.25521E5, P=1E5, N(C)=2.11631, N(N)=5.18E-4, N(O)=4.01443, N(SI)=2.69851
DEGREES OF FREEDOM 0
T= 2.058154E+03
BP(GAS)=61.542207, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=38.026721, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.871964, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 27 FROM STAGE 3
H=-8.09533E5, P=1E5, N(C)=1.65304, N(N)=3.6E-4, N(O)=3.7293, N(SI)=2.87754
DEGREES OF FREEDOM 0
T= 2.083905E+03
BP(GAS)=67.268068, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=35.329239, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,

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      BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.743144, BP(SI_L)=0, BP(SI_S)=0,
      BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION    27 FROM STAGE      4
H=10900.9, P=1E5, N(C)=0.881116, N(N)=2E-4, N(O)=1.92211, N(SI)=1.84217
DEGREES OF FREEDOM 0
T= 2.238945E+03
BP(GAS)=70.602347, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0, BP(C1S11_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
BP(SI_L)=22.472838, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION    28 FROM STAGE      1
H=-9.92907E5, P=1E5, N(C)=2.89418, N(N)=6.784E-4, N(O)=3.82457,
      N(SI)=1.73042
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.423286, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=23.401312, BP(CRISTOBALITE)=68.458959, BP(DIAMOND)=0,
BP(GRAPHITE)=9.2761374, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION    28 FROM STAGE      2
H=-9.25308E5, P=1E5, N(C)=2.10564, N(N)=5.18E-4, N(O)=4.01288, N(SI)=2.70763
DEGREES OF FREEDOM 0
T= 2.059046E+03
BP(GAS)=61.622967, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=38.032171, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.888879, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION    28 FROM STAGE      3
H=-8.09954E5, P=1E5, N(C)=1.65342, N(N)=3.6E-4, N(O)=3.73095, N(SI)=2.87876
DEGREES OF FREEDOM 0
T= 2.083910E+03
BP(GAS)=67.29288, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=35.338637, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.774212, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION    28 FROM STAGE      4
H=10503.9, P=1E5, N(C)=0.881351, N(N)=2E-4, N(O)=1.92315, N(SI)=1.84292
DEGREES OF FREEDOM 0
T= 2.235247E+03
BP(GAS)=70.643174, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0, BP(C1S11_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
BP(SI_L)=22.472477, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION    29 FROM STAGE      1
H=-9.92684E5, P=1E5, N(C)=2.88557, N(N)=6.784E-4, N(O)=3.82302,
      N(SI)=1.73749
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.435345, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=23.724241, BP(CRISTOBALITE)=68.399659, BP(DIAMOND)=0,
BP(GRAPHITE)=9.0708202, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION    29 FROM STAGE      2
H=-9.25125E5, P=1E5, N(C)=2.09675, N(N)=5.18E-4, N(O)=4.01156, N(SI)=2.71519
DEGREES OF FREEDOM 0
T= 2.059777E+03
BP(GAS)=61.689367, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=38.036539, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.902395, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION    29 FROM STAGE      3
H=-8.10275E5, P=1E5, N(C)=1.65372, N(N)=3.6E-4, N(O)=3.73223, N(SI)=2.8797
DEGREES OF FREEDOM 0
T= 2.083913E+03
BP(GAS)=67.312611, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=35.345811, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.797852, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION    29 FROM STAGE      4
H=10201.8, P=1E5, N(C)=0.88153, N(N)=2E-4, N(O)=1.92393, N(SI)=1.8435
DEGREES OF FREEDOM 0
T= 2.232430E+03
BP(GAS)=70.674247, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0, BP(C1S11_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
BP(SI_L)=22.472217, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION    30 FROM STAGE      1
H=-9.92498E5, P=1E5, N(C)=2.8784, N(N)=6.784E-4, N(O)=3.82172, N(SI)=1.74335
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.444615, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=23.99212, BP(CRISTOBALITE)=68.350461, BP(DIAMOND)=0,
BP(GRAPHITE)=8.900504, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION    30 FROM STAGE      2
H=-9.2497E5, P=1E5, N(C)=2.08938, N(N)=5.18E-4, N(O)=4.01043, N(SI)=2.72144
DEGREES OF FREEDOM 0
T= 2.060375E+03
BP(GAS)=61.743864, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=38.040041, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.913208, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION    30 FROM STAGE      3
H=-8.10519E5, P=1E5, N(C)=1.65395, N(N)=3.6E-4, N(O)=3.73322, N(SI)=2.88044
DEGREES OF FREEDOM 0
T= 2.083916E+03
BP(GAS)=67.328322, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=35.351285, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.815841, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION    30 FROM STAGE      4

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H=9971.98, P=1E5, N(C)=0.881666, N(N)=2E-4, N(O)=1.92453, N(SI)=1.84393
DEGREES OF FREEDOM 0
T= 2.230286E+03
BP(GAS)=70.697899, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
BP(SI_L)=22.472028, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 31 FROM STAGE 1
H=-9.92343E5, P=1E5, N(C)=2.87245, N(N)=6.784E-4, N(O)=3.82061,
N(SI)=1.74821
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.451748, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=24.213745, BP(CRISTOBALITE)=68.309748, BP(DIAMOND)=0,
BP(GRAPHITE)=8.7595952, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 31 FROM STAGE 2
H=-9.24838E5, P=1E5, N(C)=2.08327, N(N)=5.18E-4, N(O)=4.00947, N(SI)=2.72659
DEGREES OF FREEDOM 0
T= 2.060864E+03
BP(GAS)=61.788519, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=38.04285, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.921863, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 31 FROM STAGE 3
H=-8.10706E5, P=1E5, N(C)=1.65413, N(N)=3.6E-4, N(O)=3.73399, N(SI)=2.88101
DEGREES OF FREEDOM 0
T= 2.083919E+03
BP(GAS)=67.340845, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=35.355459, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.829531, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 31 FROM STAGE 4
H=9797.08, P=1E5, N(C)=0.88177, N(N)=2E-4, N(O)=1.92499, N(SI)=1.84426
DEGREES OF FREEDOM 0
T= 2.228654E+03
BP(GAS)=70.715902, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
BP(SI_L)=22.471889, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 32 FROM STAGE 1
H=-9.92213E5, P=1E5, N(C)=2.86752, N(N)=6.784E-4, N(O)=3.81969,
N(SI)=1.75221
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.457241, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=24.396675, BP(CRISTOBALITE)=68.276134, BP(DIAMOND)=0,
BP(GRAPHITE)=8.6432877, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 32 FROM STAGE 2
H=-9.24728E5, P=1E5, N(C)=2.07822, N(N)=5.18E-4, N(O)=4.00867, N(SI)=2.73083
DEGREES OF FREEDOM 0
T= 2.061265E+03
BP(GAS)=61.825057, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=38.045105, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.928798, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 32 FROM STAGE 3
H=-8.10849E5, P=1E5, N(C)=1.65427, N(N)=3.6E-4, N(O)=3.73458, N(SI)=2.88145
DEGREES OF FREEDOM 0
T= 2.083921E+03
BP(GAS)=67.350836, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=35.35864, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.83995, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 32 FROM STAGE 4
H=9663.98, P=1E5, N(C)=0.88185, N(N)=2E-4, N(O)=1.92533, N(SI)=1.84452
DEGREES OF FREEDOM 0
T= 2.227411E+03
BP(GAS)=70.729605, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
BP(SI_L)=22.471786, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 33 FROM STAGE 1
H=-9.92106E5, P=1E5, N(C)=2.86345, N(N)=6.784E-4, N(O)=3.81892,
N(SI)=1.75551
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.461476, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=24.547354, BP(CRISTOBALITE)=68.248438, BP(DIAMOND)=0,
BP(GRAPHITE)=8.5474847, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 33 FROM STAGE 2
H=-9.24635E5, P=1E5, N(C)=2.07406, N(N)=5.18E-4, N(O)=4.008, N(SI)=2.73432
DEGREES OF FREEDOM 0
T= 2.061592E+03
BP(GAS)=61.854916, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=38.046916, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.934356, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 33 FROM STAGE 3
H=-8.10958E5, P=1E5, N(C)=1.65438, N(N)=3.6E-4, N(O)=3.73504, N(SI)=2.88179
DEGREES OF FREEDOM 0
T= 2.083922E+03
BP(GAS)=67.358815, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=35.361063, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.84788, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 33 FROM STAGE 4
H=9562.69, P=1E5, N(C)=0.88191, N(N)=2E-4, N(O)=1.9256, N(SI)=1.84471
DEGREES OF FREEDOM 0

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T= 2.226466E+03
BP(GAS)=70.740036, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0, BP(C1S11_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
BP(SI_L)=22.471709, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 34 FROM STAGE 1
H=-9.92018E5, P=1E5, N(C)=2.8601, N(N)=6.784E-4, N(O)=3.81828, N(SI)=1.75822
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.464743, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=24.671238, BP(CRISTOBALITE)=68.225659, BP(DIAMOND)=0,
BP(GRAPHITE)=8.4687171, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 34 FROM STAGE 2
H=-9.24557E5, P=1E5, N(C)=2.07064, N(N)=5.18E-4, N(O)=4.00744, N(SI)=2.73718
DEGREES OF FREEDOM 0
T= 2.061859E+03
BP(GAS)=61.879288, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=38.04837, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.938815, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 34 FROM STAGE 3
H=-8.11041E5, P=1E5, N(C)=1.65446, N(N)=3.6E-4, N(O)=3.7354, N(SI)=2.88206
DEGREES OF FREEDOM 0
T= 2.083924E+03
BP(GAS)=67.36519, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=35.362909, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.853916, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 34 FROM STAGE 4
H=9485.6, P=1E5, N(C)=0.881956, N(N)=2E-4, N(O)=1.9258, N(SI)=1.84486
DEGREES OF FREEDOM 0
T= 2.225746E+03
BP(GAS)=70.747975, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0, BP(C1S11_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
BP(SI_L)=22.471651, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 35 FROM STAGE 1
H=-9.91944E5, P=1E5, N(C)=2.85734, N(N)=6.784E-4, N(O)=3.81775,
N(SI)=1.76044
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.467267, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=24.772923, BP(CRISTOBALITE)=68.206956, BP(DIAMOND)=0,
BP(GRAPHITE)=8.404063, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 35 FROM STAGE 2
H=-9.24493E5, P=1E5, N(C)=2.06783, N(N)=5.18E-4, N(O)=4.00698, N(SI)=2.73952
DEGREES OF FREEDOM 0
T= 2.062077E+03
BP(GAS)=61.89916, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=38.049539, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.942393, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 35 FROM STAGE 3
H=-8.11105E5, P=1E5, N(C)=1.65453, N(N)=3.6E-4, N(O)=3.73568, N(SI)=2.88226
DEGREES OF FREEDOM 0
T= 2.083924E+03
BP(GAS)=67.370289, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=35.364315, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.85851, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 35 FROM STAGE 4
H=9426.93, P=1E5, N(C)=0.881991, N(N)=2E-4, N(O)=1.92595, N(SI)=1.84497
DEGREES OF FREEDOM 0
T= 2.225198E+03
BP(GAS)=70.754019, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0, BP(C1S11_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
BP(SI_L)=22.471608, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 36 FROM STAGE 1
H=-9.91884E5, P=1E5, N(C)=2.85508, N(N)=6.784E-4, N(O)=3.8173, N(SI)=1.76227
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.469217, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=24.856262, BP(CRISTOBALITE)=68.191622, BP(DIAMOND)=0,
BP(GRAPHITE)=8.3510729, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 36 FROM STAGE 2
H=-9.24439E5, P=1E5, N(C)=2.06553, N(N)=5.18E-4, N(O)=4.00659, N(SI)=2.74144
DEGREES OF FREEDOM 0
T= 2.062255E+03
BP(GAS)=61.915348, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=38.050478, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.945266, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 36 FROM STAGE 3
H=-8.11153E5, P=1E5, N(C)=1.65458, N(N)=3.6E-4, N(O)=3.7359, N(SI)=2.88243
DEGREES OF FREEDOM 0
T= 2.083925E+03
BP(GAS)=67.374368, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=35.365386, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.862006, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 36 FROM STAGE 4
H=9382.28, P=1E5, N(C)=0.882018, N(N)=2E-4, N(O)=1.92607, N(SI)=1.84505
DEGREES OF FREEDOM 0
T= 2.224780E+03
BP(GAS)=70.758618, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0, BP(C1S11_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
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BP(SI_L)=22.471575, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 37 FROM STAGE 1
H=-9.91834E5, P=1E5, N(C)=2.85322, N(N)=6.784E-4, N(O)=3.81694,
N(SI)=1.76376
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.470726, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=24.924473, BP(CRISTOBALITE)=68.179066, BP(DIAMOND)=0,
BP(GRAPHITE)=8.3077016, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 37 FROM STAGE 2
H=-9.24394E5, P=1E5, N(C)=2.06364, N(N)=5.18E-4, N(O)=4.00627, N(SI)=2.743
DEGREES OF FREEDOM 0
T= 2.062401E+03
BP(GAS)=61.928524, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=38.051234, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.947572, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 37 FROM STAGE 3
H=-8.11191E5, P=1E5, N(C)=1.65462, N(N)=3.6E-4, N(O)=3.73607, N(SI)=2.88255
DEGREES OF FREEDOM 0
T= 2.083926E+03
BP(GAS)=67.377634, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=35.366201, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.864666, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 37 FROM STAGE 4
H=9348.31, P=1E5, N(C)=0.882038, N(N)=2E-4, N(O)=1.92616, N(SI)=1.84512
DEGREES OF FREEDOM 0
T= 2.224463E+03
BP(GAS)=70.762119, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
BP(SI_L)=22.47155, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 38 FROM STAGE 1
H=-9.91794E5, P=1E5, N(C)=2.8517, N(N)=6.784E-4, N(O)=3.81664, N(SI)=1.76498
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.471894, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=24.980232, BP(CRISTOBALITE)=68.168799, BP(DIAMOND)=0,
BP(GRAPHITE)=8.2722466, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 38 FROM STAGE 2
H=-9.24358E5, P=1E5, N(C)=2.0621, N(N)=5.18E-4, N(O)=4.00601, N(SI)=2.74428
DEGREES OF FREEDOM 0
T= 2.062519E+03
BP(GAS)=61.939239, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=38.051841, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.949425, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 38 FROM STAGE 3
H=-8.11219E5, P=1E5, N(C)=1.65465, N(N)=3.6E-4, N(O)=3.7362, N(SI)=2.88265
DEGREES OF FREEDOM 0
T= 2.083926E+03
BP(GAS)=67.38025, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=35.366821, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.866691, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 38 FROM STAGE 4
H=9322.46, P=1E5, N(C)=0.882054, N(N)=2E-4, N(O)=1.92623, N(SI)=1.84517
DEGREES OF FREEDOM 0
T= 2.224222E+03
BP(GAS)=70.764782, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
BP(SI_L)=22.471532, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 39 FROM STAGE 1
H=-9.9176E5, P=1E5, N(C)=2.85046, N(N)=6.784E-4, N(O)=3.81639, N(SI)=1.76598
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.472799, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=25.025761, BP(CRISTOBALITE)=68.160413, BP(DIAMOND)=0,
BP(GRAPHITE)=8.2432958, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 39 FROM STAGE 2
H=-9.24327E5, P=1E5, N(C)=2.06084, N(N)=5.18E-4, N(O)=4.00579, N(SI)=2.74533
DEGREES OF FREEDOM 0
T= 2.062616E+03
BP(GAS)=61.947946, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=38.052329, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.950914, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 39 FROM STAGE 3
H=-8.11241E5, P=1E5, N(C)=1.65467, N(N)=3.6E-4, N(O)=3.73631, N(SI)=2.88273
DEGREES OF FREEDOM 0
T= 2.083927E+03
BP(GAS)=67.382345, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=35.367293, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.868232, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 39 FROM STAGE 4
H=9302.8, P=1E5, N(C)=0.882065, N(N)=2E-4, N(O)=1.92628, N(SI)=1.8452
DEGREES OF FREEDOM 0
T= 2.224038E+03
BP(GAS)=70.766809, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
BP(SI_L)=22.471517, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 40 FROM STAGE 1

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H=-9.91733E5, P=1E5, N(C)=2.84944, N(N)=6.784E-4, N(O)=3.81619,
N(SI)=1.76679
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.4735, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=25.0629, BP(CRISTOBALITE)=68.15357, BP(DIAMOND)=0,
BP(GRAPHITE)=8.2196802, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 40 FROM STAGE 2
H=-9.24302E5, P=1E5, N(C)=2.05981, N(N)=5.18E-4, N(O)=4.00561, N(SI)=2.74618
DEGREES OF FREEDOM 0
T= 2.062694E+03
BP(GAS)=61.955017, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=38.052722, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.95211, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 40 FROM STAGE 3
H=-8.11257E5, P=1E5, N(C)=1.65469, N(N)=3.6E-4, N(O)=3.73639, N(SI)=2.88279
DEGREES OF FREEDOM 0
T= 2.083927E+03
BP(GAS)=67.384025, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=35.367653, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.869403, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 40 FROM STAGE 4
H=9287.84, P=1E5, N(C)=0.882074, N(N)=2E-4, N(O)=1.92632, N(SI)=1.84523
DEGREES OF FREEDOM 0
T= 2.223898E+03
BP(GAS)=70.768351, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
BP(SI_L)=22.471507, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 41 FROM STAGE 1
H=-9.9171E5, P=1E5, N(C)=2.84862, N(N)=6.784E-4, N(O)=3.81602, N(SI)=1.76745
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.474045, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=25.093165, BP(CRISTOBALITE)=68.147991, BP(DIAMOND)=0,
BP(GRAPHITE)=8.2004349, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 41 FROM STAGE 2
H=-9.24282E5, P=1E5, N(C)=2.05898, N(N)=5.18E-4, N(O)=4.00547, N(SI)=2.74687
DEGREES OF FREEDOM 0
T= 2.062758E+03
BP(GAS)=61.960755, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=38.053038, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.953071, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 41 FROM STAGE 3
H=-8.1127E5, P=1E5, N(C)=1.65471, N(N)=3.6E-4, N(O)=3.73645, N(SI)=2.88283
DEGREES OF FREEDOM 0
T= 2.083927E+03
BP(GAS)=67.385371, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=35.367926, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.870295, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 41 FROM STAGE 4
H=9276.47, P=1E5, N(C)=0.882081, N(N)=2E-4, N(O)=1.92635, N(SI)=1.84525
DEGREES OF FREEDOM 0
T= 2.223792E+03
BP(GAS)=70.769524, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
BP(SI_L)=22.471498, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 42 FROM STAGE 1
H=-9.91692E5, P=1E5, N(C)=2.84794, N(N)=6.784E-4, N(O)=3.81589,
N(SI)=1.76799
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.474468, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=25.117807, BP(CRISTOBALITE)=68.143448, BP(DIAMOND)=0,
BP(GRAPHITE)=8.1847648, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 42 FROM STAGE 2
H=-9.24265E5, P=1E5, N(C)=2.05829, N(N)=5.18E-4, N(O)=4.00535, N(SI)=2.74743
DEGREES OF FREEDOM 0
T= 2.062810E+03
BP(GAS)=61.96541, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=38.053292, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.953844, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 42 FROM STAGE 3
H=-8.1128E5, P=1E5, N(C)=1.65472, N(N)=3.6E-4, N(O)=3.7365, N(SI)=2.88287
DEGREES OF FREEDOM 0
T= 2.083928E+03
BP(GAS)=67.386451, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0,
BP(C1SI1_BETA)=35.368134, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.870973, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 42 FROM STAGE 4
H=9267.82, P=1E5, N(C)=0.882086, N(N)=2E-4, N(O)=1.92637, N(SI)=1.84527
DEGREES OF FREEDOM 0
T= 2.223711E+03
BP(GAS)=70.770415, BP(BETA_QUARTZ)=0, BP(C1SI1_ALPHA)=0, BP(C1SI1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
BP(SI_L)=22.471492, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 43 FROM STAGE 1
H=-9.91677E5, P=1E5, N(C)=2.84739, N(N)=6.784E-4, N(O)=3.81578,
N(SI)=1.76843
DEGREES OF FREEDOM 0

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T= 1.785827E+03
BP(GAS)=43.474796, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=25.137856, BP(CRISTOBALITE)=68.13975, BP(DIAMOND)=0,
BP(GRAPHITE)=8.1720159, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0, BP(TRIDYMITTE_S3)=0
>>> DATA AT ITERATION 43 FROM STAGE 2
H=-9.24251E5, P=1E5, N(C)=2.05774, N(N)=5.18E-4, N(O)=4.00525, N(SI)=2.74789
DEGREES OF FREEDOM 0
T= 2.062852E+03
BP(GAS)=61.969183, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=38.053497, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=65.954465, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0, BP(TRIDYMITTE_S3)=0
>>> DATA AT ITERATION 43 FROM STAGE 3
H=-8.11287E5, P=1E5, N(C)=1.65473, N(N)=3.6E-4, N(O)=3.73654, N(SI)=2.8829
DEGREES OF FREEDOM 0
T= 2.083928E+03
BP(GAS)=67.387317, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=35.368292, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=57.871488, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0, BP(TRIDYMITTE_S3)=0
>>> DATA AT ITERATION 43 FROM STAGE 4
H=9261.25, P=1E5, N(C)=0.88209, N(N)=2E-4, N(O)=1.92638, N(SI)=1.84528
DEGREES OF FREEDOM 0
T= 2.223650E+03
BP(GAS)=70.771093, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0, BP(C1Si1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4Si3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0,
BP(SI_L)=22.471487, BP(SI_S)=0, BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0,
BP(TRIDYMITTE_S3)=0
=====
>>> DATA AT ITERATION 44 FROM STAGE 1
H=-9.91665E5, P=1E5, N(C)=2.84694, N(N)=6.784E-4, N(O)=3.81569,
N(SI)=1.76878
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.475052, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=25.154154, BP(CRISTOBALITE)=68.136743, BP(DIAMOND)=0,
BP(GRAPHITE)=8.1616514, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0, BP(TRIDYMITTE_S3)=0
>>> DATA AT ITERATION 44 FROM STAGE 2
H=-9.2424E5, P=1E5, N(C)=2.05729, N(N)=5.18E-4, N(O)=4.00517, N(SI)=2.74826
DEGREES OF FREEDOM 0
T= 2.062886E+03
BP(GAS)=61.972241, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=38.053661, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=65.954965, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0, BP(TRIDYMITTE_S3)=0
>>> DATA AT ITERATION 44 FROM STAGE 3
H=-8.11293E5, P=1E5, N(C)=1.65474, N(N)=3.6E-4, N(O)=3.73657, N(SI)=2.88292
DEGREES OF FREEDOM 0
T= 2.083928E+03
BP(GAS)=67.388011, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=35.368412, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=57.87188, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0, BP(TRIDYMITTE_S3)=0
>>> DATA AT ITERATION 44 FROM STAGE 4
H=9256.25, P=1E5, N(C)=0.882093, N(N)=2E-4, N(O)=1.9264, N(SI)=1.84529
DEGREES OF FREEDOM 0
T= 2.223603E+03
BP(GAS)=70.771609, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0, BP(C1Si1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4Si3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0,
BP(SI_L)=22.471484, BP(SI_S)=0, BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0,
BP(TRIDYMITTE_S3)=0
=====
>>> DATA AT ITERATION 45 FROM STAGE 1
H=-9.91655E5, P=1E5, N(C)=2.84658, N(N)=6.784E-4, N(O)=3.81561,
N(SI)=1.76907
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.475251, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=25.167395, BP(CRISTOBALITE)=68.134299, BP(DIAMOND)=0,
BP(GRAPHITE)=8.1532312, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0, BP(TRIDYMITTE_S3)=0
>>> DATA AT ITERATION 45 FROM STAGE 2
H=-9.24231E5, P=1E5, N(C)=2.05692, N(N)=5.18E-4, N(O)=4.0051, N(SI)=2.74856
DEGREES OF FREEDOM 0
T= 2.062914E+03
BP(GAS)=61.974717, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=38.053794, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=65.955366, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0, BP(TRIDYMITTE_S3)=0
>>> DATA AT ITERATION 45 FROM STAGE 3
H=-8.11297E5, P=1E5, N(C)=1.65474, N(N)=3.6E-4, N(O)=3.73659, N(SI)=2.88294
DEGREES OF FREEDOM 0
T= 2.083928E+03
BP(GAS)=67.388569, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=35.368503, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=57.872177, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0, BP(TRIDYMITTE_S3)=0
>>> DATA AT ITERATION 45 FROM STAGE 4
H=9252.46, P=1E5, N(C)=0.882096, N(N)=2E-4, N(O)=1.92641, N(SI)=1.8453
DEGREES OF FREEDOM 0
T= 2.223568E+03
BP(GAS)=70.772, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0, BP(C1Si1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4Si3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0,
BP(SI_L)=22.471481, BP(SI_S)=0, BP(TRIDYMITTE)=0, BP(TRIDYMITTE_S2)=0,
BP(TRIDYMITTE_S3)=0
=====
>>> DATA AT ITERATION 46 FROM STAGE 1
H=-9.91647E5, P=1E5, N(C)=2.84628, N(N)=6.784E-4, N(O)=3.81555,
N(SI)=1.76931
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.475405, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
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BP(C1Si1_BETA)=25.178145, BP(CRISTOBALITE)=68.132315, BP(DIAMOND)=0,
BP(GRAPHITE)=8.1463948, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 46 FROM STAGE 2
H=-9.24223E5, P=1E5, N(C)=2.05662, N(N)=5.18E-4, N(O)=4.00505, N(SI)=2.7488
DEGREES OF FREEDOM 0
T= 2.062937E+03
BP(GAS)=61.976721, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=38.0539, BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0,
BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0,
BP(SiO2_LIQUID)=65.955689, BP(SI_L)=0, BP(SI_S)=0, BP(TRIDYMITE)=0,
BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 46 FROM STAGE 3
H=-8.113E5, P=1E5, N(C)=1.65475, N(N)=3.6E-4, N(O)=3.73661, N(SI)=2.88295
DEGREES OF FREEDOM 0
T= 2.083928E+03
BP(GAS)=67.389016, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=35.368572, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=57.872403, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 46 FROM STAGE 4
H=9249.57, P=1E5, N(C)=0.882097, N(N)=2E-4, N(O)=1.92642, N(SI)=1.8453
DEGREES OF FREEDOM 0
T= 2.223541E+03
BP(GAS)=70.772298, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0, BP(C1Si1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4Si3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0,
BP(SI_L)=22.471479, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 47 FROM STAGE 1
H=-9.9164E5, P=1E5, N(C)=2.84604, N(N)=6.784E-4, N(O)=3.8155, N(SI)=1.7695
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.475526, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=25.186868, BP(CRISTOBALITE)=68.130704, BP(DIAMOND)=0,
BP(GRAPHITE)=8.1408477, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 47 FROM STAGE 2
H=-9.24217E5, P=1E5, N(C)=2.05638, N(N)=5.18E-4, N(O)=4.00501, N(SI)=2.749
DEGREES OF FREEDOM 0
T= 2.062955E+03
BP(GAS)=61.978344, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=38.053986, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=65.955949, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 47 FROM STAGE 3
H=-8.11303E5, P=1E5, N(C)=1.65475, N(N)=3.6E-4, N(O)=3.73663, N(SI)=2.88296
DEGREES OF FREEDOM 0
T= 2.083928E+03
BP(GAS)=67.389375, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=35.368625, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=57.872575, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 47 FROM STAGE 4
H=9247.39, P=1E5, N(C)=0.882099, N(N)=2E-4, N(O)=1.92642, N(SI)=1.84531
DEGREES OF FREEDOM 0
T= 2.223520E+03
BP(GAS)=70.772524, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0, BP(C1Si1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4Si3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0,
BP(SI_L)=22.471478, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 48 FROM STAGE 1
H=-9.91635E5, P=1E5, N(C)=2.84585, N(N)=6.784E-4, N(O)=3.81546,
N(SI)=1.76965
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.47562, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=25.193941, BP(CRISTOBALITE)=68.129398, BP(DIAMOND)=0,
BP(GRAPHITE)=8.1363492, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 48 FROM STAGE 2
H=-9.24212E5, P=1E5, N(C)=2.05618, N(N)=5.18E-4, N(O)=4.00497, N(SI)=2.74916
DEGREES OF FREEDOM 0
T= 2.062970E+03
BP(GAS)=61.979656, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=38.054055, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=65.956158, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 48 FROM STAGE 3
H=-8.11305E5, P=1E5, N(C)=1.65475, N(N)=3.6E-4, N(O)=3.73664, N(SI)=2.88297
DEGREES OF FREEDOM 0
T= 2.083928E+03
BP(GAS)=67.389663, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=35.368665, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=57.872705, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 48 FROM STAGE 4
H=9245.73, P=1E5, N(C)=0.8821, N(N)=2E-4, N(O)=1.92643, N(SI)=1.84531
DEGREES OF FREEDOM 0
T= 2.223505E+03
BP(GAS)=70.772695, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0, BP(C1Si1_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4Si3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0,
BP(SI_L)=22.471476, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 49 FROM STAGE 1
H=-9.91631E5, P=1E5, N(C)=2.84569, N(N)=6.784E-4, N(O)=3.81543,
N(SI)=1.76978
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.475694, BP(BETA_QUARTZ)=0, BP(C1Si1_ALPHA)=0,
BP(C1Si1_BETA)=25.199675, BP(CRISTOBALITE)=68.128339, BP(DIAMOND)=0,
BP(GRAPHITE)=8.132703, BP(GRAPHITE_L)=0, BP(N4Si3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SiO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,

```

```

      BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 49 FROM STAGE 2
H=-9.24208E5, P=1E5, N(C)=2.05603, N(N)=5.18E-4, N(O)=4.00494, N(SI)=2.74929
DEGREES OF FREEDOM 0
T= 2.062982E+03
BP(GAS)=61.980717, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=38.054111, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.956325, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 49 FROM STAGE 3
H=-8.11306E5, P=1E5, N(C)=1.65475, N(N)=3.6E-4, N(O)=3.73665, N(SI)=2.88298
DEGREES OF FREEDOM 0
T= 2.083928E+03
BP(GAS)=67.389894, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=35.368695, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.872804, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 49 FROM STAGE 4
H=9244.47, P=1E5, N(C)=0.8821, N(N)=2E-4, N(O)=1.92643, N(SI)=1.84531
DEGREES OF FREEDOM 0
T= 2.223493E+03
BP(GAS)=70.772825, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0, BP(C1S11_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
BP(SI_L)=22.471475, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
>>> DATA AT ITERATION 50 FROM STAGE 1
H=-9.91627E5, P=1E5, N(C)=2.84556, N(N)=6.784E-4, N(O)=3.8154, N(SI)=1.76988
DEGREES OF FREEDOM 0
T= 1.785827E+03
BP(GAS)=43.475751, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=25.204319, BP(CRISTOBALITE)=68.127481, BP(DIAMOND)=0,
BP(GRAPHITE)=8.129749, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 50 FROM STAGE 2
H=-9.24205E5, P=1E5, N(C)=2.0559, N(N)=5.18E-4, N(O)=4.00492, N(SI)=2.7494
DEGREES OF FREEDOM 0
T= 2.062992E+03
BP(GAS)=61.981574, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=38.054155, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=65.95646, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 50 FROM STAGE 3
H=-8.11307E5, P=1E5, N(C)=1.65476, N(N)=3.6E-4, N(O)=3.73665, N(SI)=2.88298
DEGREES OF FREEDOM 0
T= 2.083928E+03
BP(GAS)=67.39008, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0,
BP(C1S11_BETA)=35.368718, BP(CRISTOBALITE)=0, BP(DIAMOND)=0,
BP(GRAPHITE)=0, BP(GRAPHITE_L)=0, BP(N4SI3_S)=0, BP(QUARTZ)=0,
BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=57.872879, BP(SI_L)=0, BP(SI_S)=0,
BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0, BP(TRIDYMITE_S3)=0
>>> DATA AT ITERATION 50 FROM STAGE 4
H=9243.51, P=1E5, N(C)=0.882101, N(N)=2E-4, N(O)=1.92643, N(SI)=1.84532
DEGREES OF FREEDOM 0
T= 2.223484E+03
BP(GAS)=70.772924, BP(BETA_QUARTZ)=0, BP(C1S11_ALPHA)=0, BP(C1S11_BETA)=0,
BP(CRISTOBALITE)=0, BP(DIAMOND)=0, BP(GRAPHITE)=0, BP(GRAPHITE_L)=0,
BP(N4SI3_S)=0, BP(QUARTZ)=0, BP(QUARTZ_S2)=0, BP(SIO2_LIQUID)=0,
BP(SI_L)=22.471475, BP(SI_S)=0, BP(TRIDYMITE)=0, BP(TRIDYMITE_S2)=0,
BP(TRIDYMITE_S3)=0
=====
REACTOR: @@ Currently no nice output is provided in this module. Use POLY-3
REACTOR: @@ to list the constitution in each segment
REACTOR: GO P-3
POLY_3: L-E
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
Output from POLY-3, equilibrium = 1004, label A0 , database: SSUB5

Conditions:
H=9243.51, P=1E5, N(C)=0.882101, N(N)=2E-4, N(O)=1.92643, N(SI)=1.84532
DEGREES OF FREEDOM 0

Temperature 2223.48 K ( 1950.33 C), Pressure 1.000000E+05
Number of moles of components 4.65405E+00, Mass in grams 9.32444E+01
Total Gibbs energy -1.35902E+06, Enthalpy 9.24351E+03, Volume 3.56321E-01

Component      Moles      W-Fraction  Activity   Potential  Ref.stat
C                8.8210E-01  1.1363E-01  5.0909E-03 -9.7618E+04 SER
N                2.0000E-04  3.0044E-05  8.4815E-09 -3.4359E+05 SER
O                1.9264E+00  3.3054E-01  1.4658E-13 -5.4632E+05 SER
SI              1.8453E+00  5.5581E-01  1.5640E-03 -1.1944E+05 SER

GAS              Status ENTERED      Driving force  0.0000E+00
Moles 3.8539E+00, Mass 7.0773E+01, Volume fraction 1.0000E+00 Mass fractions:
O 4.35491E-01 SI 4.14766E-01 C 1.49703E-01 N 3.95829E-05
Constitution:
O1S11 5.41812E-01 C1O2 2.03424E-05 C 2.35255E-10 O2 9.66134E-14
C1O1 4.57645E-01 O2S11 1.70445E-06 N1O1 7.37237E-11
SI 4.69570E-04 C1S11 3.44134E-09 C3 4.10874E-12
N2 5.18835E-05 O 9.67006E-10 C2 3.46774E-12

SI L            Status ENTERED      Driving force  0.0000E+00
Moles 8.0012E-01, Mass 2.2471E+01, Volume fraction 0.0000E+00 Mass fractions:
SI 1.00000E+00 C 0.00000E+00 O 0.00000E+00 N 0.00000E+00
POLY_3: @@ This equilibrium is valid for the fourth segment. Note it is
POLY_3: @@ identified with number 1004. The other have numbers 1001, 1002 and 1003.
POLY_3: @@ Good luck for future work with this!
POLY_3: go sys
SYS: set-inter
SYS:

```

About Software (build 9533) running on WinNT 64-bit wordlength  
 Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118  
 License library version: 8.5.1.0017  
 Linked: Mon May 16 09:31:44 2016

**SYS:**SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex25\tcex25.TCM"**SYS:** set-echo

**SYS:** @@ Simulation of steel refining

**SYS:** @@

**SYS:** @@

**SYS:** @@ Raw iron used to produce steel usually has very high carbon and

**SYS:** @@ silicon content. Oxygen is thus blown into the furnace to burn off

**SYS:** @@ carbon. Lime (CaO) is added to form a slag with silica, and the slag

**SYS:** @@ can be removed. Alloying elements, such as Mn, Ni, Cr and V are added

**SYS:** @@ to produce desired steel. Since the reaction between oxygen and

**SYS:** @@ carbon will increase the temperature, scrap iron is added in order to

**SYS:** @@ keep the temperature constant (we assume the furnace is isolated

**SYS:** @@ and no heat is lost to the environment). This is a typical steel

**SYS:** @@ refining process.

**SYS:** @@

**SYS:** @@ This example simulates blowing oxygen into a liquid steel of one

**SYS:** @@ metric ton (1e6 grams) with 4 w/o C, 2 w/o Si and 1 w/o Mn. 100 moles

**SYS:** @@ of CaO (equivalent to 5.6 kg) is added. Keeping the enthalpy constant

**SYS:** @@ is the way to simulate the isolation of the furnace. The oxygen

**SYS:** @@ will react with carbon and increase the temperature. After blowing

**SYS:** @@ a certain amount of oxygen, scrap iron is added to keep the temperature

**SYS:** @@ constant.

**SYS:** @@

**SYS:** set-log ex25,,,

**SYS:** go da

... the command in full is GOTO\_MODULE

THERMODYNAMIC DATABASE module

Current database: Steels/Fe-Alloys v8.0

VA DEFINED

L12\_FCC

B2\_BCC

B2\_VACANCY

HIGH\_SIGMA

DICTRA\_FCC\_A1 REJECTED

**TDB\_TCFE8:** @@ In this example we use data from the slag database

**TDB\_TCFE8:** sw slag3

... the command in full is SWITCH\_DATABASE

Current database: Fe-containing Slag v3.2

FE

O DEFINED

FEOLIQ REJECTED

**TDB\_SLAG3:** d-sys ca si mn c

... the command in full is DEFINE\_SYSTEM

CA

SI

MN

C DEFINED

**TDB\_SLAG3:** l-sys

... the command in full is LIST\_SYSTEM

**ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:** CONSTITUENT

GAS:G :C C2 C3 C4 C5 C60 C101 C102 C201 C302 C1Si1 C1Si2 C2Si1

C5FE105 CA CA2 CA101 FE FE2 FE101 FE102 MN MN101 MN102 O O2 O3 O1Si1 O2Si1

O2Si2 SI SI2 SI3:

> The gaseous mixture is handled by the ideal gas model

FE\_LIQUID:L :C CA FE MN O SI:

> Fe-rich liquid phase (dilute solution for other elements)

SLAG:L :A0\_01\_C00C04\_12\_SiO2 A0\_01\_C00C10\_23\_FE2O3 A0\_01\_C00C16\_11\_FEO

A0\_01\_C00C22\_11\_MNO A0\_01\_C00C27\_11\_CAO A0\_01\_C04C10\_SiFe

A0\_01\_C04C16\_SiFe A0\_01\_C04C22\_SiMn A0\_01\_C04C27\_SiCa A0\_01\_C10C16\_FEFE

A0\_01\_C10C22\_FEMN A0\_01\_C10C27\_FECA A0\_01\_C16C22\_FEMN A0\_01\_C16C27\_FECA

A0\_01\_C22C27\_MNCA:

> Slag phase handled by Kapoor-Frohberg-Gaye Quasichemical Cell Model

CAO :CAO:

> This is pure CaO\_Lime phase [CaO]

FEO :FEO:

> This is pure FeO\_Wustite phase [FeO]

FE2O3 :FE2O3:

> This is pure Fe2O3\_Hematite phase [Fe2O3]

FE3O4 :FE3O4:

> This is pure Fe3O4\_Magnetite phase [Fe3O4]

MNO :MNO:

> This is pure MnO\_Manganosite phase [MnO]

SiO2\_QUARTZ :SiO2:

> This is pure SiO2\_alpha\_Quartz phase [SiO2]

SiO2\_BETA\_QUARTZ :SiO2:

> This is pure SiO2\_beta\_Quartz phase [SiO2]

SiO2\_TRIDYMIT :SiO2:

> This is pure SiO2\_Tridymite phase [SiO2]

SiO2\_CRISTOBALITE :SiO2:

> This is pure SiO2\_Christobalite phase [SiO2]

CA3O3\_SiO2 :CAO:SiO2:

> This is pure Ca3SiO5 phase [3CaO-SiO2]

CA2O2\_SiO2 :CAO:SiO2:

> This is pure Ca2SiO4 phase [2CaO-SiO2]

CA3O3\_Si2O4 :CAO:SiO2:

> This is pure Ca3Si2O7 phase [3CaO-2SiO2]

CAO\_SiO2 :CAO:SiO2:

> This is pure CaSiO3 phase [CaO-SiO2]

FE2O2\_SiO2 :FEO:SiO2:

> This is pure Fe2SiO4 phase [2FeO-SiO2]

MN2O2\_SiO2 :MNO:SiO2:

> This is pure Mn2SiO4 phase [2MnO-SiO2]

MNO\_SiO2 :MNO:SiO2:

> This is pure MnSiO3 phase [MnO-SiO2]

GRAPHITE :C:

**TDB\_SLAG3:** get

... the command in full is GET\_DATA

REINITIATING GES5 .....

ELEMENTS .....

SPECIES .....

PHASES .....

... the command in full is AMEND\_PHASE\_DESCRIPTION

... the command in full is AMEND\_PHASE\_DESCRIPTION

... the command in full is AMEND\_PHASE\_DESCRIPTION

PARAMETERS ...

FUNCTIONS ....

List of references for assessed data

'SLAG2 (2006): TCS Fe-Containing Slag Database, V2.3, owned and provided

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    by Thermo-Calc Software.'
'TCMP2 (2009): TCS Materials Processing Database, V2.5, owned and provided
    by Thermo-Calc Software.'
'Lina Kjellqvist (2012), unpublished assessments of CaO-Fe2O3 quasi-binary
system'
'Pingfang Shi (2009), unpublished assessments of Fe3O4-bearing systems. '
'Pingfang Shi (2006), unpublished assessments of SiO2-bearing systems. '
-OK-
TDB_SLAG3: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3: @@ Assume we have one ton (1e6 gram) liquid steel with a composition
POLY_3: @@ set of 4 w/o C, 2 w/o Si and 1 w/o Mn.
POLY_3: s-c t=1673,p=1e5,b(fe)=1e6,w(c)=.04,w(si)=.02,w(mn)=.01
... the command in full is SET_CONDITION
POLY_3: l-c
... the command in full is LIST_CONDITIONS
T=1673, P=1E5, B(FE)=1E6, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2
DEGREES OF FREEDOM 2
POLY_3:Hit RETURN to continue
POLY_3: @@ To remove Si, add a small amount of top slag consisting of
POLY_3: @@ pure lime (CaO), 5.6 kg equivalent to 100 moles of CaO
POLY_3: s-i-a n(cao)=100
... the command in full is SET_INPUT_AMOUNTS
POLY_3: l-c
... the command in full is LIST_CONDITIONS
T=1673, P=1E5, B(FE)=1E6, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100,
N(O)=100
DEGREES OF FREEDOM 0
POLY_3:Hit RETURN to continue
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 1277 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 1 s, total time 1 s
POLY_3: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
Output from POLY-3, equilibrium = 1, label A0 , database: SLAG3

Conditions:
T=1673, P=1E5, B(FE)=1E6, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100,
N(O)=100
DEGREES OF FREEDOM 0

Temperature 1673.00 K ( 1399.85 C), Pressure 1.000000E+05
Number of moles of components 2.26739E+04, Mass in grams 1.08130E+06
Total Gibbs energy -2.19006E+09, Enthalpy 1.32046E+09, Volume 0.00000E+00

Component      Moles      W-Fraction  Activity  Potential  Ref.stat
C                3.6010E+03  4.0000E-02  7.5454E-02 -3.5947E+04 SER
CA               1.0000E+02  3.7065E-03  1.4244E-08 -2.5131E+05 SER
FE               1.7906E+04  9.2481E-01  7.1047E-04 -1.0084E+05 SER
MN               1.9682E+02  1.0000E-02  5.1231E-06 -1.6945E+05 SER
O                1.0000E+02  1.4796E-03  6.6380E-17 -5.1817E+05 SER
SI               7.7002E+02  2.0000E-02  1.3697E-06 -1.8780E+05 SER

FE_LIQUID      Status ENTERED      Driving force  0.0000E+00
Moles 2.2474E+04, Mass 1.0757E+06, Volume fraction 0.0000E+00 Mass fractions:
FE 9.29634E-01 SI 2.01042E-02 CA 6.94868E-07
C 4.02085E-02 MN 1.00521E-02 O 2.36693E-07

CAO            Status ENTERED      Driving force  0.0000E+00
Moles 1.9995E+02, Mass 5.6064E+03, Volume fraction 0.0000E+00 Mass fractions:
CA 7.14696E-01 C 0.00000E+00 FE 0.00000E+00
O 2.85304E-01 MN 0.00000E+00 SI 0.00000E+00

CA3O3_SiO2     Status ENTERED      Driving force  0.0000E+00
Moles 1.2313E-02, Mass 3.1236E-01, Volume fraction 0.0000E+00 Mass fractions:
CA 5.26617E-01 SI 1.23010E-01 FE 0.00000E+00
O 3.50373E-01 C 0.00000E+00 MN 0.00000E+00
POLY_3:Hit RETURN to continue
POLY_3: l-st ph
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE      STATUS      DRIVING FORCE      MOLES
CAO         ENTERED      0.000000E+00      1.999545E+02
CA3O3_SiO2  ENTERED      0.000000E+00      1.231298E-02
FE_LIQUID   ENTERED      0.000000E+00      2.247397E+04
CA2O2_SiO2  ENTERED      -1.474286E-01      0.000000E+00
GRAPHITE    ENTERED      -1.870471E-01      0.000000E+00
SLAG        ENTERED      -3.278734E-01      0.000000E+00
CA3O3_SiO2  ENTERED      -4.942106E-01      0.000000E+00
CAO_SiO2    ENTERED      -1.019253E+00      0.000000E+00
GAS         ENTERED      -2.400540E+00      0.000000E+00
SiO2_TRIDYMIT  ENTERED      -3.604879E+00      0.000000E+00
SiO2_CRISTOBALITE  ENTERED      -3.605424E+00      0.000000E+00
SiO2_BETA_QUARTZ  ENTERED      -3.625809E+00      0.000000E+00
SiO2_QUARTZ   ENTERED      -3.625823E+00      0.000000E+00
ENTERED PHASES WITH DRIVING FORCE LESS THAN -3.699744E+00
MNO SiO2 MN2O2 SiO2 MNO FE2O2 SiO2 FEO FE3O4 FE2O3
POLY_3:Hit RETURN to continue
POLY_3: @@ The steel bath will be insulated so no heat disappears
POLY_3: @@ while blowing oxygen. This means that the enthalpy of the
POLY_3: @@ system is constant and the temperature may increase. Set these
POLY_3: @@ conditions
POLY_3: s-c h
... the command in full is SET_CONDITION
Value /1.32045762E+09/:
POLY_3: s-c t=None
... the command in full is SET_CONDITION
POLY_3: l-c
... the command in full is LIST_CONDITIONS
P=1E5, B(FE)=1E6, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100, N(O)=100,
H=1.32046E9
DEGREES OF FREEDOM 0
POLY_3:Hit RETURN to continue
POLY_3: @@ When we calculate now we should get exactly the same temperature
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure

```



```

Using already calculated grid
6 ITS, CPU TIME USED 1 SECONDS
POLY_3: sh t
... the command in full is SHOW_VALUE
T=1673.
POLY_3: @@ Voila! The same equilibrium calculated with different conditions
POLY_3: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
Output from POLY-3, equilibrium = 1, label A0 , database: SLAG3

Conditions:
P=1E5, B(FE)=1E6, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100, N(O)=100,
H=1.32046E9
DEGREES OF FREEDOM 0

Temperature 1673.00 K ( 1399.85 C), Pressure 1.000000E+05
Number of moles of components 2.26739E+04, Mass in grams 1.08130E+06
Total Gibbs energy -2.19006E+09, Enthalpy 1.32046E+09, Volume 0.00000E+00

Component      Moles      W-Fraction  Activity   Potential  Ref.stat
C               3.6010E+03  4.0000E-02  7.5454E-02 -3.5947E+04 SER
CA              1.0000E+02  3.7065E-03  1.4244E-08 -2.5131E+05 SER
FE              1.7906E+04  9.2481E-01  7.1047E-04 -1.0084E+05 SER
MN              1.9682E+02  1.0000E-02  5.1231E-06 -1.6945E+05 SER
O               1.0000E+02  1.4796E-03  6.6380E-17 -5.1817E+05 SER
SI              7.7002E+02  2.0000E-02  1.3697E-06 -1.8780E+05 SER

FE_LIQUID      Status ENTERED      Driving force 0.0000E+00
Moles 2.2474E+04, Mass 1.0757E+06, Volume fraction 0.0000E+00 Mass fractions:
FE 9.29634E-01 SI 2.01042E-02 CA 6.94868E-07
C 4.02085E-02 MN 1.00521E-02 O 2.36693E-07

CAO            Status ENTERED      Driving force 0.0000E+00
Moles 1.9995E+02, Mass 5.6064E+03, Volume fraction 0.0000E+00 Mass fractions:
CA 7.14696E-01 C 0.00000E+00 FE 0.00000E+00
O 2.85304E-01 MN 0.00000E+00 SI 0.00000E+00

CA3O3_SIO2     Status ENTERED      Driving force 0.0000E+00
Moles 1.2313E-02, Mass 3.1236E-01, Volume fraction 0.0000E+00 Mass fractions:
CA 5.26617E-01 SI 1.23010E-01 FE 0.00000E+00
O 3.50373E-01 C 0.00000E+00 MN 0.00000E+00
POLY_3:Hit RETURN to continue
POLY_3: @@ Now set the oxygen content as independent variable
POLY_3: @@ and blow up to 2000 moles of O (i.e. 1000 moles of O2 i.e. 22.4 m3)
POLY_3: s-a-v 1
... the command in full is SET_AXIS_VARIABLE
Condition /NONE/: n(o)
Min value /0/: 100
Max value /1/: 2000
Increment /47.5/: 100
POLY_3: save tcex25 y
... the command in full is SAVE_WORKSPACES
POLY_3: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 100.0000
...OK

Phase Region from 100.0000 for:
FE_LIQUID
CA3O3_SIO2
CAO
Global check of removing phase at 1.66663E+02
Calculated 3 equilibria

Phase Region from 166.663 for:
FE_LIQUID
CA3O3_SIO2
Global check of adding phase at 1.66799E+02
Calculated 3 equilibria

Phase Region from 166.799 for:
FE_LIQUID
CA2O2_SIO2
CA3O3_SIO2
Global check of removing phase at 2.00157E+02
Calculated 4 equilibria

Phase Region from 200.157 for:
FE_LIQUID
CA2O2_SIO2
Global check of adding phase at 2.02166E+02
Calculated 3 equilibria

Phase Region from 202.166 for:
GAS
FE_LIQUID
CA2O2_SIO2
Global test at 1.00000E+03 .... OK
Global test at 2.00000E+03 .... OK
Terminating at 2000.00
Calculated 21 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex25\tcex
25.POLY3
POLY_3: @@ Sometimes trouble here, error 1614 means all conditions not fullfilled.
POLY_3: @@ Try to start with more oxygen ...
POLY_3: read tcex25
... the command in full is READ_WORKSPACES
POLY_3:
POLY_3: s-c n(o)
... the command in full is SET_CONDITION
Value /100/: 200
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 1277 grid points in 0 s
94 ITS, CPU TIME USED 1 SECONDS
POLY_3: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: SLAG3

```

```

Conditions:
P=1E5, B(FE)=1E6, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100, N(O)=200,
H=1.32046E9
DEGREES OF FREEDOM 0

Temperature 1723.42 K ( 1450.27 C), Pressure 1.000000E+05
Number of moles of components 2.27812E+04, Mass in grams 1.08302E+06
Total Gibbs energy -2.34831E+09, Enthalpy 1.32046E+09, Volume 0.00000E+00

Component      Moles      W-Fraction  Activity   Potential  Ref.stat
C               3.6068E+03  4.0000E-02  6.5488E-02 -3.9060E+04 SER
CA             1.0000E+02  3.7006E-03  1.5356E-09 -2.9081E+05 SER
FE             1.7906E+04  9.2334E-01  6.2289E-04 -1.0577E+05 SER
MN             1.9713E+02  1.0000E-02  4.3101E-06 -1.7703E+05 SER
O              2.0000E+02  2.9545E-03  7.6249E-16 -4.9881E+05 SER
SI             7.7124E+02  2.0000E-02  1.2968E-06 -1.9424E+05 SER

FE_LIQUID      Status ENTERED      Driving force 0.0000E+00
Moles 2.2431E+04, Mass 1.0744E+06, Volume fraction 0.0000E+00 Mass fractions:
FE 9.30742E-01 SI 1.88553E-02 O 2.34486E-06
C 4.03204E-02 MN 1.00801E-02 CA 1.80134E-08

CA2O2_SIO2     Status ENTERED      Driving force 0.0000E+00
Moles 3.4836E+02, Mass 8.5714E+03, Volume fraction 0.0000E+00 Mass fractions:
CA 4.65382E-01 SI 1.63060E-01 FE 0.00000E+00
O 3.71558E-01 C 0.00000E+00 MN 0.00000E+00

CA3O3_SIO2     Status ENTERED      Driving force 0.0000E+00
Moles 1.4085E+00, Mass 3.5732E+01, Volume fraction 0.0000E+00 Mass fractions:
CA 5.26617E-01 SI 1.23010E-01 FE 0.00000E+00
O 3.50373E-01 C 0.00000E+00 MN 0.00000E+00
POLY_3:Hit RETURN to continue
POLY_3: @@ if still trouble, add that gas should be stable (gas dissolves all)
POLY_3: @@ by increasing oxygen content
POLY_3: l-st ph
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE          STATUS      DRIVING FORCE    MOLES
CA3O3_SIO2     ENTERED      0.000000E+00    1.408525E+00
CA2O2_SIO2     ENTERED      0.000000E+00    3.483550E+02
FE_LIQUID      ENTERED      0.000000E+00    2.243144E+04
SLAG           ENTERED     -1.455619E-01    0.000000E+00
CA3O3_Si2O4    ENTERED     -2.500340E-01    0.000000E+00
GRAPHITE       ENTERED     -2.698781E-01    0.000000E+00
CAO            ENTERED     -4.788199E-01    0.000000E+00
CAO_SIO2       ENTERED     -6.202161E-01    0.000000E+00
GAS            ENTERED     -1.307773E+00    0.000000E+00
SIO2_TRIDYMITTE ENTERED     -2.566026E+00    0.000000E+00
SIO2_CRISTOBALITE ENTERED     -2.566180E+00    0.000000E+00
SIO2_BETA_QUARTZ ENTERED     -2.587799E+00    0.000000E+00
SIO2_QUARTZ    ENTERED     -2.587813E+00    0.000000E+00
ENTERED PHASES WITH DRIVING FORCE LESS THAN -2.764555E+00
MNO_SIO2 MN2O2_SIO2 MNO FE2O2_SIO2 FEO FE3O4 FE2O3
POLY_3: c-st p gas
... the command in full is CHANGE_STATUS
Status: /ENTERED/:
Start value, number of moles /O/: 1
POLY_3: s-c n(o)=300
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated      1277 grid points in      0 s
37 ITS, CPU TIME USED 1 SECONDS
POLY_3: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: SLAG3

Conditions:
P=1E5, B(FE)=1E6, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100, N(O)=300,
H=1.32046E9
DEGREES OF FREEDOM 0

Temperature 1737.41 K ( 1464.26 C), Pressure 1.000000E+05
Number of moles of components 2.28885E+04, Mass in grams 1.08474E+06
Total Gibbs energy -2.42505E+09, Enthalpy 1.32046E+09, Volume 1.41396E+01

Component      Moles      W-Fraction  Activity   Potential  Ref.stat
C               3.6125E+03  4.0000E-02  5.9862E-02 -4.0675E+04 SER
CA             1.0000E+02  3.6947E-03  1.1359E-11 -3.6405E+05 SER
FE             1.7906E+04  9.2188E-01  6.0707E-04 -1.0700E+05 SER
MN             1.9745E+02  1.0000E-02  4.1965E-06 -1.7886E+05 SER
O              3.0000E+02  4.4248E-03  1.1809E-14 -4.6327E+05 SER
SI             7.7247E+02  2.0000E-02  1.2680E-06 -1.9614E+05 SER

GAS            Status ENTERED      Driving force 0.0000E+00
Moles 1.9576E+02, Mass 2.7425E+03, Volume fraction 1.0000E+00 Mass fractions:
O 5.71009E-01 MN 3.26864E-04 FE 1.77084E-05
C 4.28581E-01 SI 6.50792E-05 CA 9.33307E-08
Constitution:
C1O1 9.99604E-01 C2O1 3.60024E-11 O2 2.65004E-16
MN 1.66700E-04 FE1O1 2.16563E-11 C1SI1 1.89897E-16
C1O2 1.55481E-04 C2SI1 1.24191E-12 FE1O2 1.35522E-17
O1SI1 6.49233E-05 O 1.07250E-12 CA2 4.52820E-18
FE 8.88424E-06 CA1O1 1.56195E-13 MN1O2 4.07663E-18
CA 6.52467E-08 FE2 1.23188E-13 C5 7.36602E-20
O2SI2 4.12168E-10 C1SI2 3.31148E-14 SI3 6.62708E-20
O2SI1 2.76336E-10 C 3.19274E-14 C4 3.28485E-20
SI 2.45777E-10 C3 5.66532E-15 C5FE1O5 8.43862E-25
MN1O1 7.33238E-11 SI2 7.96419E-16 C6O 1.00000E-30
C3O2 5.29278E-11 C2 6.41588E-16 O3 1.00000E-30

FE_LIQUID      Status ENTERED      Driving force 0.0000E+00
Moles 2.2343E+04, Mass 1.0734E+06, Volume fraction 0.0000E+00 Mass fractions:
FE 9.31632E-01 SI 1.89032E-02 O 3.16069E-05
C 3.93281E-02 MN 1.01049E-02 CA 8.34231E-13

CA2O2_SIO2     Status ENTERED      Driving force 0.0000E+00
Moles 3.5000E+02, Mass 8.6118E+03, Volume fraction 0.0000E+00 Mass fractions:
CA 4.65382E-01 SI 1.63060E-01 FE 0.00000E+00
O 3.71558E-01 C 0.00000E+00 MN 0.00000E+00
POLY_3:Hit RETURN to continue
POLY_3: save tcex25 y
... the command in full is SAVE_WORKSPACES

```

This file contains results from a previous STEP or MAP command.  
The SAVE command will save the current status of the program but destroy  
the results from the previous STEP or MAP commands.

```
POLY_3: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value    300.000
...OK

Phase Region from    300.000    for:
  GAS
  FE LIQUID
  CA2O2_SIO2
Global test at    1.10000E+03 .... OK
Terminating at    2000.00
Calculated    20 equilibria

Phase Region from    300.000    for:
  GAS
  FE LIQUID
  CA2O2_SIO2
Global check of removing phase at    2.02166E+02
Calculated    3 equilibria

Phase Region from    202.166    for:
  FE LIQUID
  CA2O2_SIO2
Global check of adding phase at    2.00157E+02
Calculated    3 equilibria

Phase Region from    200.157    for:
  FE LIQUID
  CA2O2_SIO2
  CA3O3_SIO2
Global check of removing phase at    1.66799E+02
Calculated    4 equilibria

Phase Region from    166.799    for:
  FE LIQUID
  CA3O3_SIO2
Global check of adding phase at    1.66663E+02
Calculated    3 equilibria

Phase Region from    166.663    for:
  FE LIQUID
  CA3O3_SIO2
  CAO
Terminating at    100.0000
Calculated    4 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex25\tcex
25.POLY3
POLY_3:
POLY_3: @@ The calculations up to 2000 moles is saved on file. At this
POLY_3: @@ point we will change the conditions and start adding scrap in
POLY_3: @@ order to keep the temperature constant. However, the current
POLY_3: @@ equilibrium is at 100 moles of O so we must first make an
POLY_3: @@ interactive calculation at 2000 moles.
POLY_3: read tcex25
... the command in full is READ_WORKSPACES
POLY_3:
POLY_3: s-c n(o)
... the command in full is SET_CONDITION
Value /300/: 2005
POLY_3: @@ We choose the value a little bigger than 2000 moles as otherwise the
POLY_3: @@ upper limit of the previous calculation coincides with the lower limit of
POLY_3: @@ this calculation and that will cause trouble
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated    1277 grid points in    0 s
    30 ITS, CPU TIME USED    1 SECONDS
POLY_3: sh t
... the command in full is SHOW_VALUE
T=1948.7315
POLY_3: @@ We now want to keep the temperature constant by adding scrap
POLY_3: @@ Set the temperature as condition
POLY_3: s-c t
... the command in full is SET_CONDITION
Value /1948.731454/:
POLY_3:
POLY_3: l-c
... the command in full is LIST_CONDITIONS
T=1948.73, P=1E5, B(FE)=1E6, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100,
N(O)=2005, H=1.32046E9
DEGREES OF FREEDOM -1
POLY_3:Hit RETURN to continue
POLY_3: @@ we have too many conditions. Assuming the scrap is pure iron we can
POLY_3: @@ just release the condition on the amount of fe.
POLY_3: s-c b(fe)
... the command in full is SET_CONDITION
Value /1000000/: none
POLY_3: l-c
... the command in full is LIST_CONDITIONS
T=1948.73, P=1E5, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100, N(O)=2005,
H=1.32046E9
DEGREES OF FREEDOM 0
POLY_3:Hit RETURN to continue
POLY_3: @@ It is rather special to have both enthalpy
POLY_3: @@ and temperature set as conditions.
POLY_3: @@ We must change the axis limits
POLY_3: s-a-v 1
... the command in full is SET_AXIS_VARIABLE
Condition /N(O)/:
Min value /100/: 2000
Max value /2000/: 4000
Increment /50/: 100
POLY_3: @@ We must not give a save command now as that would destroy the
POLY_3: @@ results from the previous step command.
POLY_3: step normal
... the command in full is STEP_WITH_OPTIONS
```

No initial equilibrium, using default  
Step will start from axis value 2005.00  
...OK

Phase Region from 2005.00 for:

GAS  
FE\_LIQUID  
CA2O2\_SIO2

Global test at 2.80500E+03 .... OK  
Global check of adding phase at 3.77833E+03  
Calculated 20 equilibria

Phase Region from 3778.33 for:

GAS  
FE\_LIQUID  
SLAG  
CA2O2\_SIO2

Global check of removing phase at 3.87008E+03  
Calculated 4 equilibria

Phase Region from 3870.08 for:

GAS  
FE\_LIQUID  
SLAG

Terminating at 4000.00  
Calculated 5 equilibria

Phase Region from 2005.00 for:

GAS  
FE\_LIQUID  
CA2O2\_SIO2

Terminating at 2000.00  
Calculated 4 equilibria

\*\*\* Buffer saved on file:  
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex25\tcex25.POLY3

POLY\_3: @@ We shall now plot the combined results

POLY\_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

POST: @@ Use volume of added O2 as independent axis, 1 mole O2 is 0.0224 m3

POST: @@ Volume=.0224\*(moles of O2)=0.0224\*0.5\*(moles of O)

POST: enter fun vo=0.0112\*n(o);

... the command in full is ENTER\_SYMBOL

POST: s-d-a x vo

... the command in full is SET\_DIAGRAM\_AXIS

POST: s-d-a y t-c

... the command in full is SET\_DIAGRAM\_AXIS

POST: @@ Set a nicer axis text

POST: s-a-t-s x n

... the command in full is SET\_AXIS\_TEXT\_STATUS

AXIS TEXT : Volume O2 in m3

POST:

POST:

POST: set-title example 25a

POST: plot

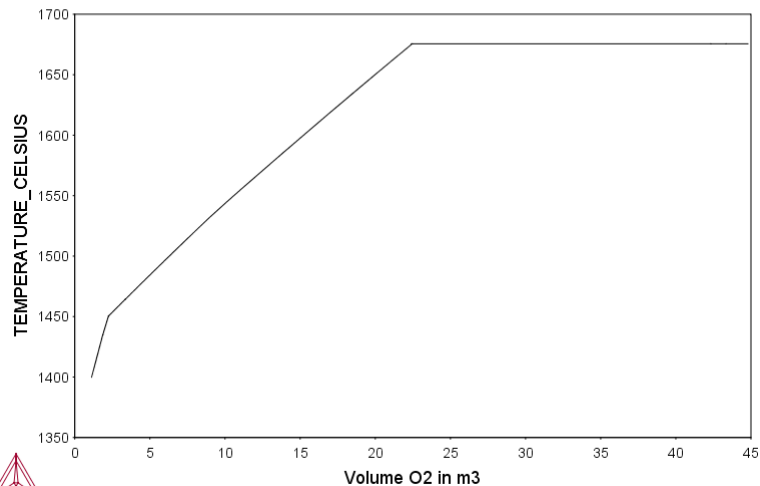
... the command in full is PLOT DIAGRAM

**example 25a**

2016.05.16.13.55.40

SLAG3: C, CA, FE, MN, O, SI

T=1948.73, P=1E5, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100, H=1.32046E9



POST:

POST:Hit RETURN to continue

POST: @@ Plot the amount of Fe (in grams!)

POST: s-d-a y b(fe)

... the command in full is SET\_DIAGRAM\_AXIS

POST: set-title example 25b

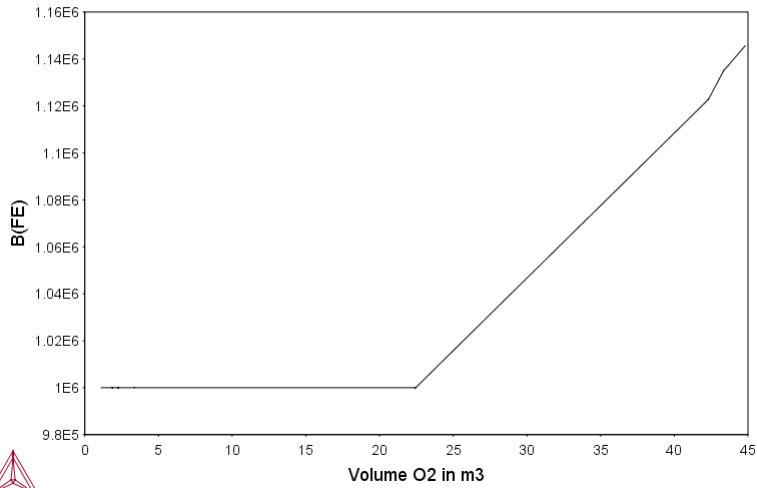
POST:

POST: plot

... the command in full is PLOT\_DIAGRAM

# example 25b

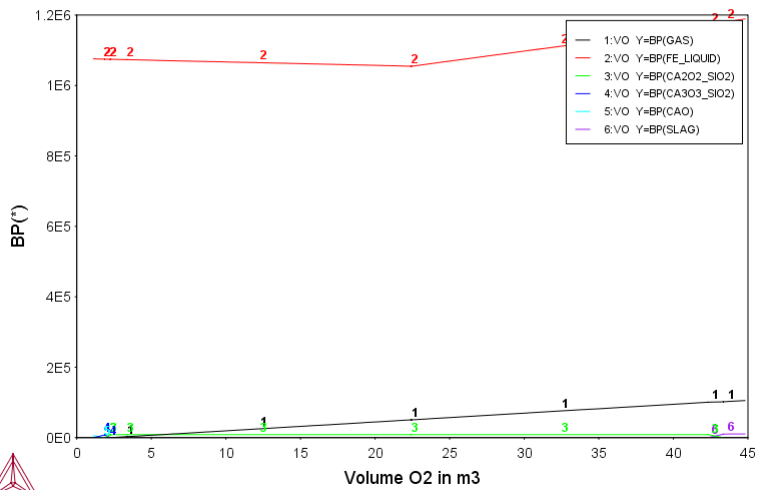
2016.05.16.13.55.41  
SLAG3: C, CA, FE, MN, O, SI  
T=1948.73, P=1E5, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100., H=1.32046E9



POST:  
POST:Hit RETURN to continue  
POST: @@ Plot the mass of all phases  
POST: s-d-a y bp(\*)  
... the command in full is SET\_DIAGRAM\_AXIS  
COLUMN NUMBER /\*/:  
POST:  
POST: set-lab D  
... the command in full is SET\_LABEL\_CURVE\_OPTION  
POST: set-title example 25c  
POST:  
POST: plot  
... the command in full is PLOT DIAGRAM

# example 25c

2016.05.16.13.55.41  
SLAG3: C, CA, FE, MN, O, SI  
T=1948.73, P=1E5, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100., H=1.32046E9



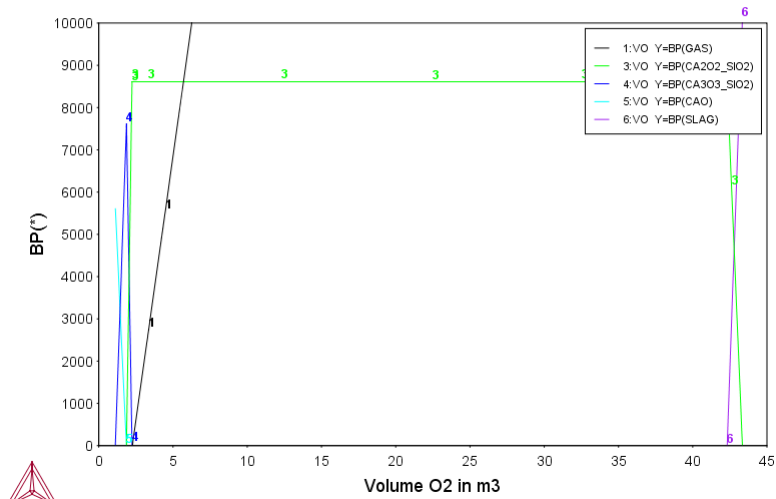
POST:  
POST:Hit RETURN to continue  
POST: @@ Scale up the slag amount. Liquid slags come at the end only.  
POST: s-s y n 0 10000  
... the command in full is SET\_SCALING\_STATUS  
POST: set-title example 25d  
POST:  
POST: plot  
... the command in full is PLOT\_DIAGRAM

# example 25d

2016.05.16 13:55:41

SLAG3: C, CA, FE, MN, O, SI

T=1948.73, P=1E5, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100., H=1.32046E9



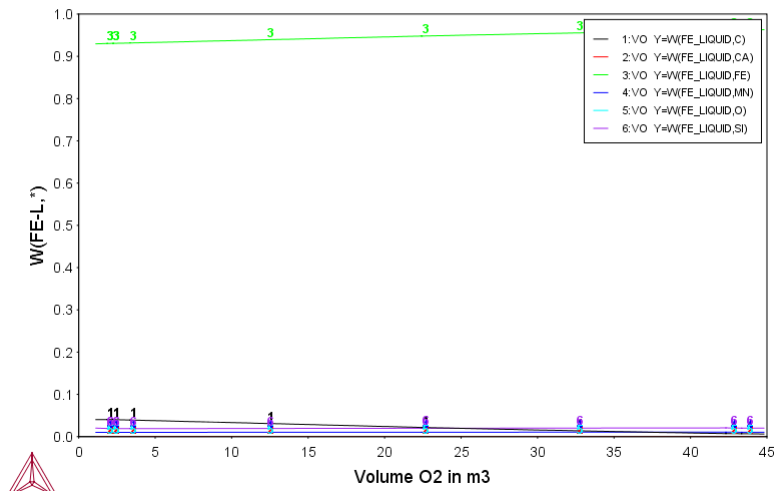
POST:  
 POST:Hit RETURN to continue  
 POST: @@ Now plot the reason for all this -- the steel composition  
 POST: s-d-a y w(fe-l,\*)  
 ... the command in full is SET\_DIAGRAM\_AXIS  
 COLUMN NUMBER /\*/:  
 POST:  
 POST: set-title example 25e  
 POST:  
 POST: plot  
 ... the command in full is PLOT DIAGRAM

# example 25e

2016.05.16 13:55:41

SLAG3: C, CA, FE, MN, O, SI

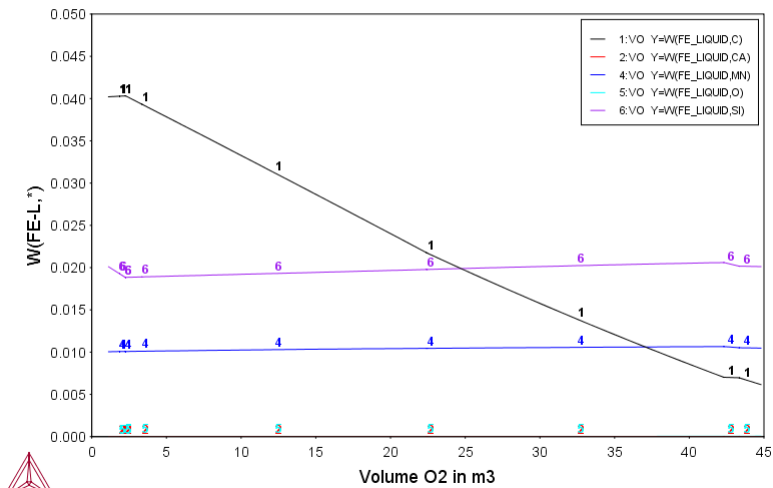
T=1948.73, P=1E5, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100., H=1.32046E9



POST:  
 POST:Hit RETURN to continue  
 POST: @@ Scale up the diagram to get the important part  
 POST: s-s y n 0.05  
 ... the command in full is SET\_SCALING\_STATUS  
 POST: set-title example 25f  
 POST:  
 POST: plot  
 ... the command in full is PLOT\_DIAGRAM

### example 25f

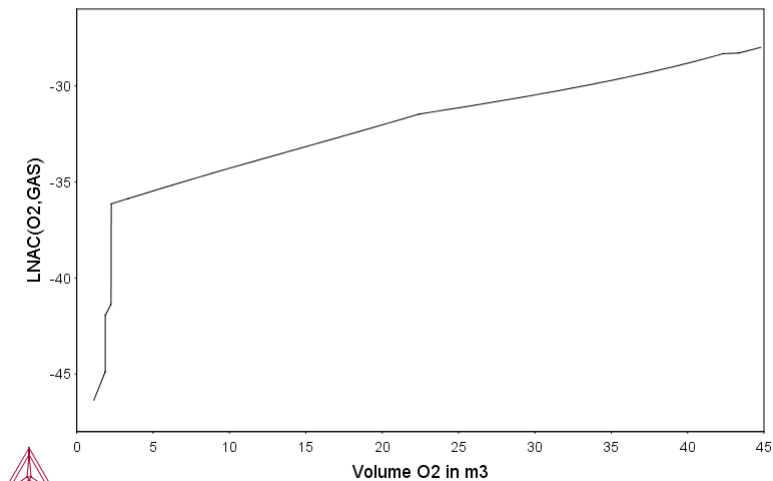
2016.05.16.13.55.42  
 SLAG3: C, CA, FE, MN, O, SI  
 T=1948.73, P=1E5, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100., H=1.32046E9



```
POST:
POST:Hit RETURN to continue
POST: @@ Finally plot the oxygen partial pressure and carbon activity.
POST: @@ For the oxygen plot LN(activity)
POST: s-d-a y lnac(o2,gas)
... the command in full is SET_DIAGRAM_AXIS
POST: set-lab none
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 25g
POST:
POST: plot
... the command in full is PLOT DIAGRAM
```

### example 25g

2016.05.16.13.55.42  
 SLAG3: C, CA, FE, MN, O, SI  
 T=1948.73, P=1E5, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100., H=1.32046E9



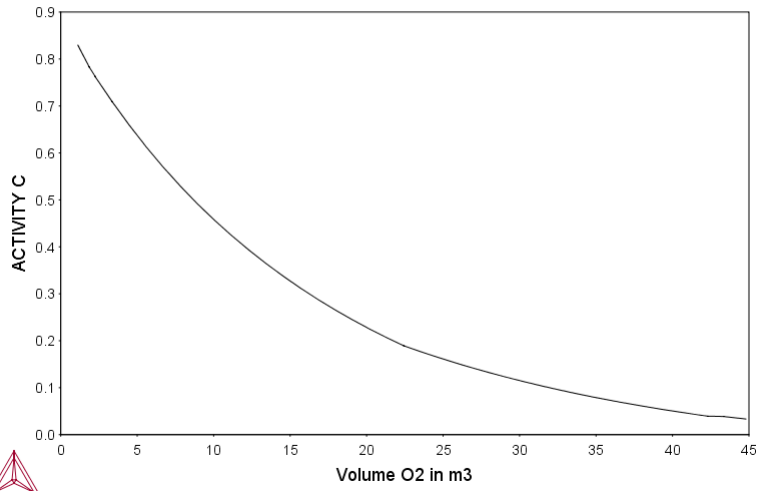
```
POST:
POST:Hit RETURN to continue
POST:
POST: @@ For carbon do not forget to set reference state
POST: set-ref-state c gra * 1e5
... the command in full is SET_REFERENCE_STATE
You should set-diagram-axis for the activity/potential after this!
POST: s-d-a y ac c
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 25h
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
```

### example 25h

2016.05.16.13.55.42

SLAG3: C, CA, FE, MN, O, SI

T=1948.73, P=1E5, W(C)=4E-2, W(SI)=2E-2, W(MN)=1E-2, N(CA)=100., H=1.32046E9



POST:

POST:Hit RETURN to continue

POST:

POST:

POST: set-inter

... the command in full is SET\_INTERACTIVE\_MODE

POST:



About Software (build 9533) running on WinNT 64-bit wordlength  
 Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118  
 License library version: 8.5.1.0017  
 Linked: Mon May 16 09:31:44 2016

SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex26\tcex26.TCM" set-echo

```
SYS: @@
SYS: @@ Plotting of the partial pressure
SYS: @@ of gas species along the solubility lines
SYS: @@ in the As-Ga Phase diagram
SYS: @@
SYS: @@ Example of plotting the partial pressures of a gas along the
SYS: @@ solubility lines in a phase diagram.
SYS: @@ The system is As-Ga.
SYS: @@ The calculation makes it possible to monitor the input gases to
SYS: @@ a process of depositing solid AsGa
SYS: @@
SYS: set-log ex26,,,,
SYS: go da
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
L12 FCC          B2_BCC          B2_VACANCY
HIGH_SIGMA      DICTRA_FCC_A1 REJECTED
TDB_TCFE8: @@ At present the data is taken from the special III-V database
TDB_TCFE8: @@ These data will eventually be incorporated in the SGTE solution database
TDB_TCFE8: sw
... the command in full is SWITCH_DATABASE
Use one of these databases

TCFE8  = Steels/Fe-Alloys v8.0
TCFE9  = Steels/Fe-Alloys v9.0 SNAPSHOT
FROST1 = FROST database v1.0
TCFE7  = Steels/Fe-Alloys v7.0
TCFE6  = Steels/Fe-Alloys v6.2
TCFE5  = Steels/Fe-Alloys v5.0
TCFE4  = Steels/Fe-Alloys v4.1
TCFE3  = Steels/Fe-Alloys v3.1
TCFE2  = Steels/Fe-Alloys v2.1
TCFE1  = Steels/Fe-Alloys v1.0
FEDAT  = TCS/TT Steels Database v1.0
TCNI9  = Ni-Alloys v9.0 SNAPSHOT
TCNI8  = Ni-Alloys v8.0
TCNI7  = Ni-Alloys v7.1
TCNI6  = Ni-Alloys v6.0
TCNI5  = Ni-Alloys v5.1
TCNI4  = Ni-Alloys v4.0
TCNI1  = Ni-Alloys v1.3
TCAL4  = Al-Alloys v4.0
TCAL3  = Al-Alloys v3.0
TCAL2  = Al-Alloys v2.0
TCAL1  = Al-Alloys v1.2
TCMG5  = Mg-Alloys v5.0 SNAPSHOT
TCMG4  = Mg-Alloys v4.0
TCMG3  = Mg-Alloys v3.0
TCMG2  = Mg-Alloys v2.0
TCMG1  = Mg-Alloys v1.1
TCTI1  = Ti-Alloys v1.0 SNAPSHOT
TCCU1  = Copper v1.0 SNAPSHOT
TCCC1  = Cemented carbide v1.0
TCHEA1 = High Entropy Alloy v1.0
SSOL5  = SGTE Alloy Solutions Database v5.0
SSOL4  = SGTE Alloy Solutions Database v4.9f
SSOL2  = SGTE Alloy Solutions Database v2.1
SSUB5  = SGTE Substances Database v5.1
SSUB4  = SGTE Substances Database v4.1
SSUB3  = SGTE Substances Database v3.3
SSUB2  = SGTE Substances Database v2.2
SNOB3  = SGTE Nobel Metal Alloys Database v3.1
SNOB2  = SGTE Nobel Metal Alloys Database v2.1
SNOB1  = SGTE Nobel Metal Alloys Database v1.2
STBC2  = SGTE Thermal Barrier Coating TDB v2.2
STBC1  = SGTE Thermal Barrier Coating TDB v1.1
SALT1  = SGTE Molten Salts Database v1.2
SNUX6  = SGTE In-Vessel Nuclear Oxide TDB v6.2
SEMC2  = TC Semi-Conductors v2.1
SLAG4  = Fe-containing Slag v4.0 snapshot
SLAG3  = Fe-containing Slag v3.2
SLAG2  = Fe-containing Slag v2.2
SLAG1  = Fe-containing Slag v1.2
TCOX7  = Metal Oxide Solutions v7.0 SNAPSHOT
TCOX6  = Metal Oxide Solutions v6.1
TCOX5  = Metal Oxide Solutions v5.1
TCOX4  = Metal Oxide Solutions v4.1
ION3   = Ionic Solutions v3.0
ION2   = Ionic Solutions v2.6
ION1   = Ionic Solutions v1.5
NOX2   = NPL Oxide Solutions Database v2.1
TCSLD3 = Solder Alloys v3.1
TCSLD2 = Solder Alloys v2.0
TCSLD1 = Solder Alloys v1.0
TCSI1  = Ultrapure Silicon v1.1
TCMP2  = Materials Processing v2.5
TCES1  = Combustion/Sintering v1.1
TCSC1  = Super Conductor v1.0
TCFC1  = SOFC Database v1.0
TCNF2  = Nuclear Fuels v2.1b
NUMT2  = Nuclear Materials v2.1
NUOX4  = Nuclear Oxides v4.2
NUTO1  = U-Zr-Si Ternary Oxides TDB v1.1
NUTA1  = Ag-Cd-In Ternary Alloys TDB v1.1
NUCL10 = ThermoData NUCLEA Alloys-oxides TDB v10.2
MEPH11 = ThermoData MEPHISTA Nuclear Fuels TDB v11
TCAQ2  = Aqueous Solution v2.5
AQS2   = TGG Aqueous Solution Database v2.5
GCE2   = TGG Geochemical/Environmental TDB v2.3
PURE5  = SGTE Unary (Pure Elements) TDB v5.1
ALDEMO = Aluminum Demo Database
FEDEMO = Iron Demo Database
```

```

NIDEMO = Nickel Demo Database
SLDEMO = Solder Demo Database
OXDEMO = Oxide Demo Database
SUBDEMO = Substance Demo Database
PTERN = Public Ternary Alloys TDB v1.3
PAQ2 = Public Aqueous Soln (SIT) TDB v2.4
PG35 = G35 Binary Semi-Conductors TDB v1.2
MOB2 = Alloys Mobility v2.4
MOB1 = Alloys Mobility v1.3
MOBFE1 = Steels/Fe-Alloys Mobility v1.0
MOBFE2 = Steels/Fe-Alloys Mobility v2.0
MOBFE3 = Steels/Fe-Alloys Mobility v3.0
MOBNI4 = Ni-Alloys Mobility v4.0
MOBNI3 = Ni-Alloys Mobility v3.1
MOBNI2 = Ni-Alloys Mobility v2.4
MOBNI1 = Ni-Alloys Mobility v1.0
MOBAL3 = Al-Alloys Mobility v3.0
MOBAL2 = Al-Alloys Mobility v2.0
MOBAL1 = Al-Alloys Mobility v1.0
MOBCU1 = Cu-Alloys Mobility v1.0 SNAPSHOT
MOBMG1 = Mg-Alloys Mobility v1.0
MOBSI1 = Si-Alloys Mobility v1.0
MOBTI1 = Ti-Alloys Mobility v1.0
MALDEMO = Al-Alloys Mobility demo database
MFEDEMO = Fe-Alloys Mobility demo database
MNIDEMO = Ni-Alloys Mobility demo database
USER = User defined Database

```

**DATABASE NAME /TCFE8/:** pg35

Current database: G35 Binary Semi-Conductors TDB v1.2

VA DEFINED

AL1G	AL2G	ALASG
ALPG	ALP2G	ALSBG

REJECTED

AS1G	ASGAG	ASING
AS2G	AS3G	AS4G

REJECTED

GA1G	GA2G	GAPG
GASBG	GASB2G	REJECTED

IN1G	IN2G	INPG
INSBG	INSB2G	REJECTED

P1G	P2G	P4G
SB1G	SB2G	SB3G

SB4G	REJECTED	
------	----------	--

**TDB\_PG35:** d-sys as ga

... the command in full is DEFINE\_SYSTEM

AS GA DEFINED

**TDB\_PG35:** @@ Reject all but the stable phases in this system

**TDB\_PG35:** rej ph /all

... the command in full is REJECT

GAS:G	LIQUID	FCC_A1
HCP_A3	FCC_B3	BCT_A5

BCT_A6	P_RED	ASP
RHOMBO_A7	ORTHO	GA_GAMMA

REJECTED

**TDB\_PG35:** rest ph liq rhom ortho fcc\_b3 gas:g

... the command in full is RESTORE

LIQUID	RHOMBO_A7	ORTHO
FCC_B3	GAS:G	RESTORED

**TDB\_PG35:** l-sys

... the command in full is LIST\_SYSTEM

**ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/:** CONSTITUENTS

GAS:G :AS1 AS2 AS3 AS4 AS1GA1 GA1 GA2:

> Gaseous mixture phase: using the Ideal EOS & Mixing Model

LIQUID :AS GA:

> Liquid mixture phase: Metallic species Al-As-Ga-In-P-Sb

FCC\_B3 :GA:AS:

> FCC\_B3 solution phase: for the complete Al-As-Ga-In-P-Sb system

RHOMBO\_A7 :AS:

> RHOMBO\_A7 solution phase: for the As-Sb binary join only

ORTHO :GA:

**TDB\_PG35:**Hit RETURN to continue

**TDB\_PG35:** get

... the command in full is GET\_DATA

REINITIATING GES5 .....

ELEMENTS .....

SPECIES .....

PHASES .....

PARAMETERS ...

FUNCTIONS ....

List of references for assessed data

'PG35 - ISC Group III-V Binary Semiconductors Database (V1.2), developed by Informal scientific Collaboration Group (Ansara I., Chatillon C., Lukas H.L., Nishizawa T., Ohtani H., Ishida K., Hillert M., Sundman B., Argent B.B., Watson A., Chart T. G., and Anderson T.), 1994, as published data [A Binary Database for III-V Compound Semiconductor Systems, Calphad, 18, 177-222] and provided by Thermo-Calc Software (May 2003/June 2008). '

-OK-

**TDB\_PG35:** go p-3

... the command in full is GOTO\_MODULE

POLY version 3.32

**POLY\_3:** @@ Set conditions at the As rich side of the system.

**POLY\_3:** @@ We want to calculate the metastable system without gas phase

**POLY\_3:** @@ but later plot the gas constitution. Thus set gas to be dormant.

**POLY\_3:** s-c t=1200 p=1e5 n=1 x(ga)=.3

... the command in full is SET\_CONDITION

**POLY\_3:** c-s p gas=dor

... the command in full is CHANGE\_STATUS

**POLY\_3:** c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Using global minimization procedure

Calculated	140 grid points in	0 s
------------	--------------------	-----

Found the set of lowest grid points in	0 s
--	-----

Calculated POLY solution	0 s, total time	0 s
--------------------------	-----------------	-----

**POLY\_3:** l-e

... the command in full is LIST\_EQUILIBRIUM

**OUTPUT TO SCREEN OR FILE /SCREEN/:**

**Options /VWCS/:** x

Output from POLY-3, equilibrium = 1, label A0 , database: PG35

```

Conditions:
T=1200, P=1E5, N=1, X(GA)=0.3
DEGREES OF FREEDOM 0

Temperature 1200.00 K ( 926.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 7.33623E+01
Total Gibbs energy -8.75968E+04, Enthalpy 1.20850E+04, Volume 0.00000E+00

Component      Moles      M-Fraction  Activity  Potential  Ref.stat
AS              7.0000E-01  7.0000E-01  1.2211E-03 -6.6929E+04 SER
GA              3.0000E-01  3.0000E-01  1.2244E-06 -1.3582E+05 SER

GAS              Status DORMANT      Driving force 8.1507E-01
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mole fractions:
AS 1.00000E+00 GA 9.09718E-11
Constitution:
AS4 9.80210E-01 AS1 2.30505E-07 GA2 1.87160E-17
AS2 1.77817E-02 GA1 3.55191E-10
AS3 2.00768E-03 AS1GA1 5.27773E-12

LIQUID           Status ENTERED      Driving force 0.0000E+00
Moles 5.0575E-01, Mass 3.7617E+01, Volume fraction 0.0000E+00 Mole fractions:
AS 8.95449E-01 GA 1.04551E-01

FCC_B3           Status ENTERED      Driving force 0.0000E+00
Moles 4.9425E-01, Mass 3.5745E+01, Volume fraction 0.0000E+00 Mole fractions:
AS 5.00000E-01 GA 5.00000E-01
POLY_3:Hit RETURN to continue
POLY_3: @@ Note that the gas would like to be stable (driving force positive)
POLY_3: @@ but it is not allowed to form as it is dormant.
POLY_3: 1-st ph
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE           STATUS      DRIVING FORCE      MOLES
LIQUID           ENTERED      0.000000E+00      5.057539E-01
FCC_B3           ENTERED      0.000000E+00      4.942461E-01
RHOMBO_A7        ENTERED      -4.059045E-01      0.000000E+00
ORTHO            ENTERED      -6.644230E+00      0.000000E+00
GAS              DORMANT      8.150658E-01
POLY_3: @@ The phase diagram is calculated with the composition and
POLY_3: @@ temperature on the axis as usual
POLY_3: s-a-v 1 x(ga)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: 1
Increment /.025/: .025
POLY_3: s-a-v 2 t
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 300
Max value /1/: 2000
Increment /42.5/: 25
POLY_3: @@ For an explanation of these symbols see below
POLY_3: ent fun pas1=0.4343*lnacr(as1,gas);
... the command in full is ENTER_SYMBOL
POLY_3: ent fun pas2=0.4343*lnacr(as2,gas);
... the command in full is ENTER_SYMBOL
POLY_3: ent fun pas3=0.4343*lnacr(as3,gas);
... the command in full is ENTER_SYMBOL
POLY_3: ent fun pas4=0.4343*lnacr(as4,gas);
... the command in full is ENTER_SYMBOL
POLY_3: ent fun pasga=0.4343*lnacr(as1ga1,gas);
... the command in full is ENTER_SYMBOL
POLY_3: ent fun pga1=0.4343*lnacr(ga1,gas);
... the command in full is ENTER_SYMBOL
POLY_3: ent tab pp
... the command in full is ENTER_SYMBOL
Variable(s): pas1 pas2 pas3 pas4 pasga pga1;
POLY_3:
POLY_3: 1-sym
... the command in full is LIST_SYMBOLS
DEFINED FUNCTIONS AND VARIABLES%
PAS1=.4343*LNACR(AS1,GAS)
PAS2=.4343*LNACR(AS2,GAS)
PAS3=.4343*LNACR(AS3,GAS)
PAS4=.4343*LNACR(AS4,GAS)
PASGA=.4343*LNACR(AS1GA1,GAS)
PGA1=.4343*LNACR(GA1,GAS)
DEFINED TABLES
PP=PAS1, PAS2, PAS3, PAS4, PASGA, PGA1
POLY_3:Hit RETURN to continue
POLY_3: ent fun dd=0.4343*dgf(gas);
... the command in full is ENTER_SYMBOL
POLY_3: ent fun qas1=log10(y(gas,as1))+dd;
... the command in full is ENTER_SYMBOL
POLY_3: ent fun qas2=log10(y(gas,as2))+dd;
... the command in full is ENTER_SYMBOL
POLY_3: ent fun qas3=log10(y(gas,as3))+dd;
... the command in full is ENTER_SYMBOL
POLY_3: ent fun qas4=log10(y(gas,as4))+dd;
... the command in full is ENTER_SYMBOL
POLY_3: ent fun qasga=log10(y(gas,as1ga1))+dd;
... the command in full is ENTER_SYMBOL
POLY_3: ent fun qga1=log10(y(gas,ga1))+dd;
... the command in full is ENTER_SYMBOL
POLY_3: ent tab qq
... the command in full is ENTER_SYMBOL
Variable(s): qas1 qas2 qas3 qas4 qasga qga1;
POLY_3:
POLY_3: ent fun it=1000/T;
... the command in full is ENTER_SYMBOL
POLY_3: save tcex26 y
... the command in full is SAVE_WORKSPACES
POLY_3: 1-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*DPF(GAS)
QAS1= LOG10(Y(GAS,AS1) )+DD
QAS2= LOG10(Y(GAS,AS2) )+DD

```

```

QAS3= LOG10(Y(GAS,AS3) )+DD
QAS4= LOG10(Y(GAS,AS4) )+DD
QASGA= LOG10(Y(GAS,AS1GA1) )+DD
QGA1= LOG10(Y(GAS,GA1) )+DD
IT=1000/T
DEFINED TABLES
PP=PAS1, PAS2, PAS3, PAS4, PASGA, PGA1
QQ=QAS1, QAS2, QAS3, QAS4, QASGA, QGA1
POLY_3:Hit RETURN to continue
POLY_3: @@ Map follows all lines in the phase diagram
POLY_3: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

Phase region boundary 1 at: 2.500E-01 3.100E+02
** FCC_B3
RHOMBO_A7
Calculated.. 2 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 2.500E-01 3.000E+02
** FCC_B3
RHOMBO_A7
Calculated.. 32 equilibria

Phase region boundary 3 at: 2.500E-01 1.067E+03
** FCC_B3
** LIQUID
RHOMBO_A7

Phase region boundary 4 at: 2.345E-02 1.067E+03
** LIQUID
RHOMBO_A7
Calculated 10 equilibria

Phase region boundary 5 at: 2.734E-01 1.067E+03
FCC_B3
** LIQUID
Calculated. 101 equilibria

Phase region boundary 6 at: 7.500E-01 3.029E+02
FCC_B3
** LIQUID
** ORTHO

Phase region boundary 7 at: 7.500E-01 3.029E+02
FCC_B3
** ORTHO
Calculated.. 2 equilibria
Terminating at axis limit.

Phase region boundary 8 at: 1.000E+00 3.029E+02
LIQUID
** ORTHO
Calculated 12 equilibria

Phase region boundary 9 at: 2.500E-01 3.100E+02
** FCC_B3
RHOMBO_A7
Calculated. 32 equilibria
Terminating at known equilibrium

Phase region boundary 10 at: 2.500E-01 3.100E+02
** FCC_B3
RHOMBO_A7
Calculated.. 2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 11 at: 2.500E-01 3.100E+02

```

```

** FCC_B3
  RHOMBO_A7
Calculated.          32 equilibria
Terminating at known equilibrium

Phase region boundary 12 at:  2.500E-01  3.100E+02
** FCC_B3
  RHOMBO_A7
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 13 at:  2.500E-01  3.100E+02
** FCC_B3
  RHOMBO_A7
Calculated.          32 equilibria
Terminating at known equilibrium

Phase region boundary 14 at:  7.500E-01  3.100E+02
** FCC_B3
  LIQUID
Calculated.          2 equilibria
Terminating at known equilibrium

Phase region boundary 15 at:  7.500E-01  3.100E+02
** FCC_B3
  LIQUID
Calculated.         100 equilibria
Terminating at known equilibrium

Phase region boundary 16 at:  7.500E-01  3.100E+02
** FCC_B3
  LIQUID
Calculated.          2 equilibria
Terminating at known equilibrium

Phase region boundary 17 at:  7.500E-01  3.100E+02
** FCC_B3
  LIQUID
Calculated.         100 equilibria
Terminating at known equilibrium

Phase region boundary 18 at:  7.500E-01  3.100E+02
** FCC_B3
  LIQUID
Calculated.          2 equilibria
Terminating at known equilibrium

Phase region boundary 19 at:  7.500E-01  3.100E+02
** FCC_B3
  LIQUID
Calculated.         100 equilibria
Terminating at known equilibrium

Phase region boundary 20 at:  2.500E-01  8.700E+02
** FCC_B3
  RHOMBO_A7
Calculated..         24 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 21 at:  2.500E-01  8.700E+02
** FCC_B3
  RHOMBO_A7
Calculated.          9 equilibria
Terminating at known equilibrium

Phase region boundary 22 at:  7.492E-01  8.700E+02
** FCC_B3
  LIQUID
Calculated.         24 equilibria
Terminating at known equilibrium

Phase region boundary 23 at:  7.492E-01  8.700E+02
** FCC_B3
  LIQUID
Calculated.         81 equilibria
Terminating at known equilibrium

Phase region boundary 24 at:  3.939E-01  1.430E+03
** FCC_B3
  LIQUID
Calculated.         18 equilibria
Terminating at known equilibrium

Phase region boundary 25 at:  3.939E-01  1.430E+03
** FCC_B3
  LIQUID
Calculated.         87 equilibria
Terminating at known equilibrium

Phase region boundary 26 at:  6.143E-01  1.430E+03
** FCC_B3
  LIQUID
Calculated.         50 equilibria
Terminating at known equilibrium

Phase region boundary 27 at:  6.143E-01  1.430E+03
** FCC_B3
  LIQUID
Calculated.         55 equilibria
Terminating at known equilibrium

Phase region boundary 28 at:  5.000E-03  1.086E+03
  LIQUID
** RHOMBO_A7
Calculated           15 equilibria

Phase region boundary 29 at:  5.000E-03  1.086E+03
  LIQUID
** RHOMBO_A7
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 30 at:  4.183E-01  1.463E+03
** FCC_B3

```

```

LIQUID
Calculated.                21 equilibria
Terminating at known equilibrium

Phase region boundary 31 at:  4.183E-01  1.463E+03
** FCC_B3
LIQUID
Calculated.                67 equilibria
Terminating at known equilibrium

Phase region boundary 32 at:  5.817E-01  1.468E+03
** FCC_B3
LIQUID
Calculated.                34 equilibria
Terminating at known equilibrium

Phase region boundary 33 at:  5.817E-01  1.468E+03
** FCC_B3
LIQUID
Calculated.                54 equilibria
Terminating at known equilibrium

Phase region boundary 34 at:  7.450E-01  9.995E+02
** FCC_B3
LIQUID
Calculated.                74 equilibria
Terminating at known equilibrium

Phase region boundary 35 at:  7.450E-01  9.995E+02
** FCC_B3
LIQUID
Calculated.                29 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex26\tcex
26.POLY3
CPU time for mapping                0 seconds
POLY_3: @@ Now we plot this in the post processor
POLY_3: post

```

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

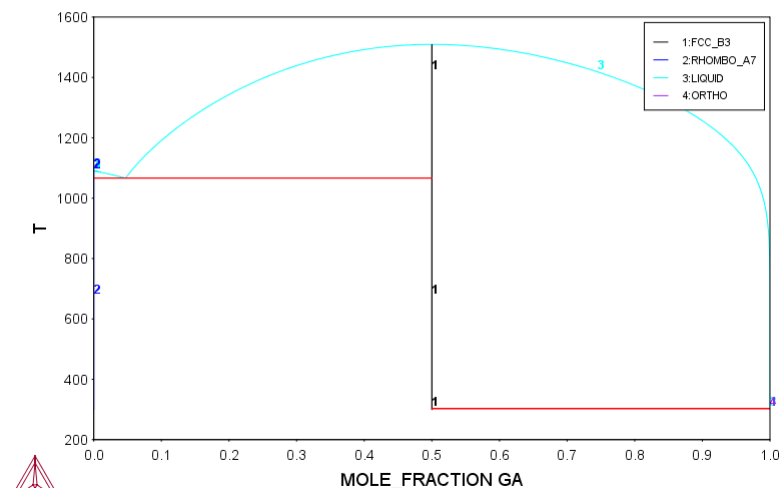
```

POST: s-d-a x m-f ga
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t
... the command in full is SET_DIAGRAM_AXIS
POST: s-l d
... the command in full is SET_LABEL_CURVE_OPTION
POST:
POST: set-title example 26a
POST: plot
... the command in full is PLOT DIAGRAM

```

example 26a

2016.05.16.13.57.49  
PG35:AS,GA  
P=1E5,N=1



```

POST:
POST: Hit RETURN to continue
POST: @@ This is the traditional phase diagram.
POST: @@
POST: @@ Now those who work with this system is interested to know the
POST: @@ partial pressures of the different gas species along the
POST: @@ solubility lines. As Thermo-Calc saves the complete description of
POST: @@ all tie-lines calculated in a MAP or STEP command, even for
POST: @@ dormant phases, we can now plot these.
POST: @@ The partial pressures of a species in the gas is equal to the
POST: @@ fraction of that species if the gas is stable (Dalton's law)
POST: @@ If the gas is not stable one must add the driving force per
POST: @@ formula unit of the gas (the formula unit depends on the species)
POST: @@
POST: @@ We can obtain directly the activity of a gas species using the
POST: @@ state variable acr(species,gas) which will have as
POST: @@ reference state a pure gas of the species itself. The state variable
POST: @@ lnacr(species,gas) is the natural logarithm of this quantity. To make
POST: @@ it into log10 one must multiply by 0.4343
POST: @@
POST: s-d-a y pp
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: @@ plot again the inverse of temperature
POST: s-d-a x it
... the command in full is SET_DIAGRAM_AXIS

```

```

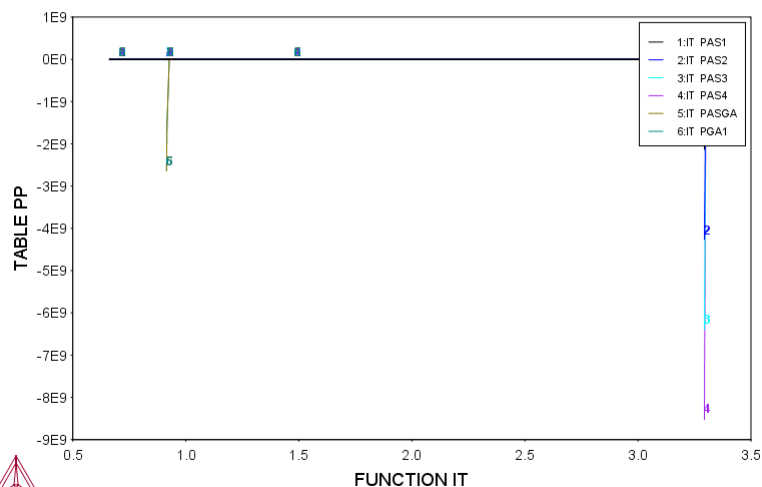
POST: l-sy
... the command in full is LIST_SYMBOLS
DEFINED CONSTANTS
ZERO=0
DEFINED FUNCTIONS AND VARIABLES%
PAS1=.4343*LNACR(AS1,GAS)
PAS2=.4343*LNACR(AS2,GAS)
PAS3=.4343*LNACR(AS3,GAS)
PAS4=.4343*LNACR(AS4,GAS)
PASGA=.4343*LNACR(AS1GA1,GAS)
PGA1=.4343*LNACR(GA1,GAS)
DD=.4343*DGF(GAS)
QAS1= LOG10(Y(GAS,AS1) )+DD
QAS2= LOG10(Y(GAS,AS2) )+DD
QAS3= LOG10(Y(GAS,AS3) )+DD
QAS4= LOG10(Y(GAS,AS4) )+DD
QASGA= LOG10(Y(GAS,AS1GA1) )+DD
QGA1= LOG10(Y(GAS,GA1) )+DD
IT=1000/T
TEMP_C=T-273.15
DEFINED TABLES
PP=PAS1, PAS2, PAS3, PAS4, PASGA, PGA1
QQ=QAS1, QAS2, QAS3, QAS4, QASGA, QGA1

```

POST: set-title example 26b

POST: plot  
... the command in full is PLOT DIAGRAM  
example 26b

2016.05.16.13.57.50  
PG35: AS, GA  
P=1E5, N=1

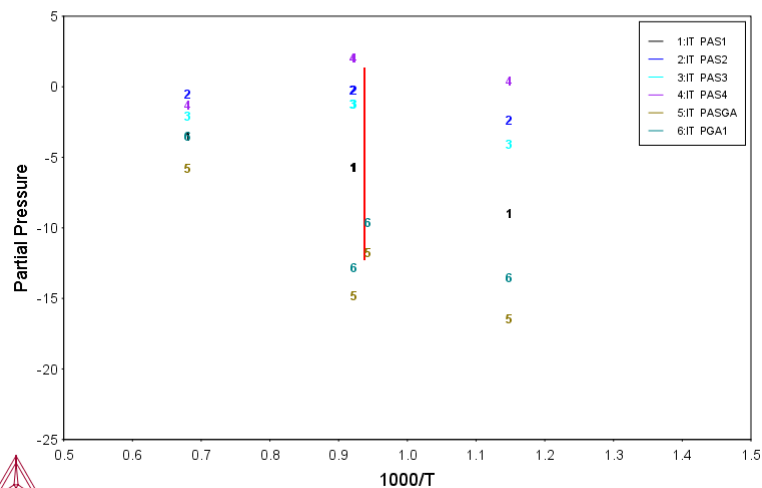


```

POST:
POST:Hit RETURN to continue
POST: @@ Now make the plot readable by adding axis text and labels
POST: s-s x n 0.5 1.5
... the command in full is SET_SCALING_STATUS
POST: s-s y n -25 5
... the command in full is SET_SCALING_STATUS
POST: s-a-text x n 1000/T
... the command in full is SET_AXIS_TEXT_STATUS
POST: s-a-text y n Partial Pressure
... the command in full is SET_AXIS_TEXT_STATUS
POST: s-lab d
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 26c
POST:
POST: plot
... the command in full is PLOT DIAGRAM
example 26c

```

2016.05.16.13.57.50  
PG35: AS, GA  
P=1E5, N=1



```

POST:
POST: set-interactive
... the command in full is SET_INTERACTIVE_MODE
POST:

```





tcex27

```
AboutSYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex27\tcex27.TCM"SYS: set-echo
SYS: @@
SYS: @@
SYS: @@ Example of CVD calculation
SYS: @@
SYS: @@
SYS: @@ Get data from database
SYS: set-log ex27,,,,
SYS: go da
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
LI2_FCC          B2_BCC          B2_VACANCY
HIGH_SIGMA      DICTRA_FCC_A1   REJECTED
TDB_TCFE8: sw ssb5
... the command in full is SWITCH_DATABASE
Current database: SGTE Substances Database v5.1

VA DEFINED
TDB_SSUB5:
TDB_SSUB5: d-sys h cl ar w si
... the command in full is DEFINE_SYSTEM
H          CL          AR
W          SI   DEFINED
TDB_SSUB5: get
... the command in full is GET_DATA
REINITIATING GES5 .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

AR1<G> HULTGREN SELECTED VAL 1973 SGTE **
AR1<G> Ar<G>
ARGON <GAS>
STANDARD STATE : CODATA KEY VALUE .
CL1<G> T.C.R.A.S. Class: 1
CL1<G> Cl<G>
CHLORINE <MONATOMIC GAS>
CL10W2<G> JANAF THERMOCHEMICAL TABLES SGTE
CL10W2<G> W2Cl10<G>
TUNGSTEN PENTACHLORIDE <GAS>
PUBLISHED BY JANAF AT 12/66
CL1H1<G> T.C.R.A.S. Class: 1
CL1H1<G> HCl<G>
HYDROGEN CHLORIDE <GAS>
CL1H1S11<G> T.C.R.A.S. Class: 5
CL1H1S11<G> SiHCl<G>
CL1H3S11<G> R.W.T.H.-91 SGTE **
CL1H3S11<G> SiH3Cl<G>
MOLWT(G/M): 66.5630
CL1S11<G> T.C.R.A.S. Class: 1
CL1S11<G> SiCl<G>
SILICON MONOCHLORIDE <GAS>
CL1W1<G> T.C.R.A.S. Class: 3
CL1W1<G> WCl<G>
TUNGSTEN MONOCHLORIDE <GAS>
CL2<G> T.C.R.A.S. Class: 1
CL2<G> Cl2<G> Chlorine gas
CHLORINE <DIATOMIC GAS>
CL2H2S11<G> THERMODATA 01/93
CL2H2S11<G> SiH2Cl2<G>
DICHLOROSILANE
28/01/93 DICHLOROSILANE.
CL2S11<G> T.C.R.A.S. Class: 5
CL2S11<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
CL3H1S11<G> THERMODATA 01/93
CL3H1S11<G> SiHCl3<G>
28/01/93
CL3S11<G> T.C.R.A.S. Class: 6
CL3S11<G> SiCl3<G>
SILICON TRICHLORIDE <GAS>
CL3W1<G> T.C.R.A.S. Class: 6
CL3W1<G> WCl3<G>
CL4S11<G> T.C.R.A.S. Class: 6
CL4S11<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>
H1S11<G> T.C.R.A.S. Class: 2
H1S11<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
H2S11<G> T.C.R.A.S. Class: 6
H2S11<G> SiH2<G>
H3S11<G> T.C.R.A.S. Class: 5
```

```

H3SI1<G> SiH3<G>
H4SI1<G> JANAF 1978; ASSESSMENT DATED 6/76 SGTE
H4SI1<G> SiH4<G>
SILANE <GAS>
H6SI2<G> THERMODATA 01/93
H6SI2<G> Si2H6<G>
DISILANE <GAS>
28/01/93
SI1<G> T.C.R.A.S. Class: 1
SI1<G> Si<G>
SILICON <GAS>
SI2<G> T.C.R.A.S. Class: 5
SI2<G> Si2<G>
SILICON <DIATOMIC GAS>
SI3<G> T.C.R.A.S. Class: 6
SI3<G> Si3<G>
SILICON <TRIATOMIC GAS>
W1<G> T.C.R.A.S. Class: 4
W1<G> W<G>
TUNGSTEN <GAS>
CL2W1 JANAF THERMOCHEMICAL TABLES SGTE **
CL2W1 WC12
TUNGSTEN DICHLORIDE
PUBLISHED BY JANAF AT 12/66
Decomposes and sublimates to complex vapour at about 860K.
CL3W1 T.C.R.A.S. Class: 7
CL3W1 WC13
CL4SI1<L> N.P.L. SGTE **
CL4SI1_Liquid SiCl4_Liquid
SILICON TETRACHLORIDE
ESTIM.COEF.FOR CP .MELTING PT. AT 203.15 K. LF=1850(#100)CAL/MOL FOR
GAS
SEE SI1CL4<G> ABOVE 331 K.
CL4W1 JANAF THERMOCHEMICAL TABLES SGTE
CL4W1 WC14
TUNGSTEN TETRACHLORIDE
PUBLISHED BY JANAF AT 12/66
Decomposes at 771K to WC12(s) and WC15(g).
CL5W1 JANAF THERMOCHEMICAL TABLES SGTE
CL5W1 WC15
TUNGSTEN PENTACHLORIDE
PUBLISHED BY JANAF AT 12/66
CL6W1 THERMODATA 01/93
CL6W1 WC16
TUNGSTEN HEXACHLORIDE
28/01/93 Tb = 613.6 K
H6SI2 THERMODATA 06/86 BK
H6SI2 Si2H6
SI2W1 VAHLAS ET AL **
SI2W1 WSi2
from Vahlas et al Calphad 13(3) (1989) 273
SI3W5 VAHLAS ET AL **
SI3W5 WSi3
from Vahlas et al Calphad 13(3) (1989) 273
SI1 JANAF THERMOCHEMICAL TABLES SGTE **
SI1 Si
SILICON
PUBLISHED BY JANAF AT 12/66 . MPT FROM NBS BULL. (IPTS-68)
--U.D. 31/10/85
W1 S.G.T.E. **
W1 W
Data from SGTE Unary DB
-OK-
TDB_SSUB5: @@
TDB_SSUB5: @@ Calculations are made in POLY-3 module
TDB_SSUB5: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3: @@
POLY_3: @@ In poly-3 you define new components
POLY_3: def-com ar cl4w1 cl2h2si1 h2 cl1h1
... the command in full is DEFINE_COMPONENTS
POLY_3: l-st c
... the command in full is LIST_STATUS
*** STATUS FOR ALL COMPONENTS
COMPONENT          STATUS      REF. STATE      T(K)          P(Pa)
VA                  ENTERED      SER
AR                  ENTERED      SER
CL4W1               ENTERED      SER
CL2H2SI1            ENTERED      SER
H2                  ENTERED      SER
CL1H1               ENTERED      SER
POLY_3:Hit RETURN to continue
POLY_3: @@
POLY_3: @@ Set conditions for input of gases. This may be tricky. The best
POLY_3: @@ is probably to set amounts equal to moles/minutes or something
POLY_3: @@ like that. In this case we had initial partial pressures of
POLY_3: @@ argon 0.9 atm, WCL4 1e-5..0.1 SiH2Cl2 1e-5..0.1 unknown presure of H2.
POLY_3: @@ Should be no addition of HCl nor Cl but added a small addition of
POLY_3: @@ cl1h1 to get equilibrium to converge.
POLY_3: s-c n=1 x(ar)=.9 x(cl2h2si1)=1e-3 x(cl4w1)=.001 x(cl1h1)=1e-12
... the command in full is SET_CONDITION
POLY_3: @@
POLY_3: @@ At the reaction zone T=1000 and total pressure is 1 atm
POLY_3: s-c t=1000 p=101325
... the command in full is SET_CONDITION
POLY_3: l-c
... the command in full is LIST_CONDITIONS
N=1, X(AR)=0.9, X(CL2H2SI1)=1E-3, X(CL4W1)=1E-3, X(CL1H1)=1E-12, T=1000,
P=1.01325E5
DEGREES OF FREEDOM 0
POLY_3: @@
POLY_3: @@ Save what we have done so far on a file if something happens ...
POLY_3: @@ and then calculate and list the results
POLY_3: save tcex27 y
... the command in full is SAVE_WORKSPACES
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated          482 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution          0 s, total time          0 s
POLY_3: l-e

```

```

... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
Output from POLY-3, equilibrium =      1, label A0  , database: SSUB5

Conditions:
N=1, X(AR)=0.9, X(CL2H2SI1)=1E-3, X(CL4W1)=1E-3, X(CL1H1)=1E-12, T=1000,
P=1.01325E5
DEGREES OF FREEDOM 0

Temperature 1000.00 K ( 726.85 C), Pressure 1.013250E+05
Number of moles of components 1.00000E+00, Mass in grams 3.65774E+01
Total Gibbs energy -1.67561E+05, Enthalpy 1.45855E+04, Volume 8.21892E-02

Component      Moles      W-Fraction  Activity  Potential  Ref.stat
AR              9.0000E-01  9.8293E-01  2.0867E-09 -1.6619E+05 SER
CL4W1           1.0000E-03  8.9034E-03  8.9672E-57 -1.0730E+06 SER
CL2H2SI1        1.0000E-03  2.7615E-03  1.5207E-40 -7.6231E+05 SER
H2              9.8000E-02  5.4008E-03  2.4479E-09 -1.6486E+05 SER
CL1H1           1.0021E-12  9.9886E-13  1.9600E-18 -3.3901E+05 SER

GAS              Status ENTERED      Driving force 0.0000E+00
Moles 1.0016E+00, Mass 3.6377E+01, Volume fraction 1.0000E+00 Mass fractions:
AR              9.8835E-01  CL1H1      5.2120E-03  CL4W1      1.3133E-10
H2              5.3198E-03  CL2H2SI1   1.1106E-03
Constitution:
AR              8.9856E-01  CL          3.0307E-11  H1SI1      1.5452E-17
H2              9.6553E-02  CL1H1SI1    2.2561E-11  SI         2.7019E-19
CL1H1           4.4853E-03  CL2W1       1.4646E-11  H6SI2      1.3683E-22
CL4SI1          3.1622E-04  H4SI1       6.0328E-12  CL5W1      4.3779E-24
CL3H1SI1        7.8199E-05  CL1SI1      1.4137E-12  SI2        1.2646E-26
CL1H3SI1        4.2979E-06  CL2         6.1572E-15  CL1W1      1.3560E-30
CL2H2SI1        3.5004E-07  H3SI1       4.2211E-16  SI3        1.1560E-30
CL2SI1          2.9018E-07  H2SI1       3.8009E-16  W          1.0000E-30
CL3SI1          3.2949E-09  CL4W1       1.1260E-16  CL10W2     1.0000E-30
H               7.0122E-10  CL3W1       1.6206E-17  CL6W1      1.0000E-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           1.6226E+00  H2          2.0087E-02  CL1H1      -9.4467E-01
CL2H2SI1        3.0196E-01  AR          0.0000E+00
POLY 3:Hit RETURN to continue
POLY 3: @@ Now set axis to vary along the input amounts of WCL4 and SiH2Cl2.
POLY 3: @@ Use logarithmic step as the magnitudes varies a lot.
POLY 3: @@ Note that a limit equal to zero should not be used with log.axis!
POLY 3: s-a-v 1 x(cl2h2si)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 1e-8
Max value /1/: 0.02
Increment /4.999975E-04/: 2.0*
Logarithmic step set
POLY 3: s-a-v 2 x(cl4w)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 1e-8
Max value /1/: 0.02
Increment /4.999975E-04/: 2.0*
Logarithmic step set
POLY 3: @@ Add with both direction and continuation ">" to be sure to get all lines
POLY 3: add
... the command in full is ADD_INITIAL_EQUILIBRIUM
Direction /Default/: 2>
POLY 3: add -2>
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY 3: l-ax
... the command in full is LIST_AXIS_VARIABLE
Axis No 1: X(CL2H2SI1)      Min: 1E-8      Max: 2E-2      Inc: 2*
Axis No 2: X(CL4W1)        Min: 1E-8      Max: 2E-2      Inc: 2*
POLY 3: li-in
... the command in full is LIST_INITIAL_EQUILIBRIA
No 1 +2> N=1., X(AR)=0.9, X(CL2H2SI1)=1E-3, X(CL4W1)=1E-3,
X(CL1H1)=1.0022937E-12, T=1000, P=101325
No 2 -2> N=1., X(AR)=0.9, X(CL2H2SI1)=1E-3, X(CL4W1)=1E-3,
X(CL1H1)=1.0021064E-12, T=1000, P=101325
POLY 3:Hit RETURN to continue
POLY 3: @@
POLY 3: @@ save again with the start point before mapping
POLY 3: save tcex27 y
... the command in full is SAVE_WORKSPACES
POLY 3: map
Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Tie-lines not in the plane of calculation
Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18

Phase region boundary 1 at: 1.435E-02 1.970E-03
GAS
SI2W1_S
** SI_S
Calculated 68 equilibria

Phase region boundary 2 at: 1.435E-02 1.970E-03
GAS
SI2W1_S

```

```

** SI_S
Calculated..                2 equilibria
Terminating at axis limit.

Phase region boundary  3 at:  2.000E-02  2.810E-03
  GAS
  SI2W1_S
** SI_S
Calculated                  70 equilibria

Phase region boundary  4 at:  9.344E-03  1.970E-03
  GAS
  SI2W1_S
** SI3W5_S
Calculated                  79 equilibria

Phase region boundary  5 at:  9.344E-03  1.970E-03
  GAS
  SI2W1_S
** SI3W5_S
Calculated..                3 equilibria
Terminating at axis limit.

Phase region boundary  6 at:  2.000E-02  3.793E-03
  GAS
  SI2W1_S
** SI3W5_S
Calculated                  84 equilibria

Phase region boundary  7 at:  4.095E-03  1.970E-03
  GAS
  SI2W1_S
  SI3W5_S
Calculated                  65 equilibria

Phase region boundary  8 at:  4.095E-03  1.970E-03
  GAS
  SI2W1_S
  SI3W5_S
Calculated..                4 equilibria
Terminating at axis limit.

Phase region boundary  9 at:  2.000E-02  7.114E-03
  GAS
  SI2W1_S
  SI3W5_S
Calculated                  70 equilibria

Phase region boundary 10 at:  2.938E-03  1.970E-03
  GAS
  SI3W5_S
** W_S
Calculated                  83 equilibria

Phase region boundary 11 at:  2.938E-03  1.970E-03
  GAS
  SI3W5_S
** W_S
Calculated..                4 equilibria
Terminating at axis limit.

Phase region boundary 12 at:  2.000E-02  7.879E-03
  GAS
  SI3W5_S
** W_S
Calculated                  84 equilibria

Phase region boundary 13 at:  1.000E-03  1.970E-03
  GAS
  SI3W5_S
  W_S
Calculated                  89 equilibria

Phase region boundary 14 at:  1.000E-03  1.970E-03
  GAS
  SI3W5_S
  W_S
Calculated..                6 equilibria
Terminating at axis limit.

Phase region boundary 15 at:  2.000E-02  1.266E-02
  GAS
  SI3W5_S
  W_S
Calculated                  99 equilibria

Phase region boundary 16 at:  1.000E-03  1.970E-03
  GAS
  SI3W5_S
  W_S
Calculated                  36 equilibria

Phase region boundary 17 at:  1.000E-03  1.970E-03
  GAS
  SI3W5_S
  W_S
Calculated..                7 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 18 at:  1.000E-03  1.037E-03
  GAS
  SI3W5_S
** W_S
Calculated                  35 equilibria

Phase region boundary 19 at:  1.000E-03  1.037E-03
  GAS
  SI3W5_S
** W_S
Calculated..                6 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 20 at:  1.000E-03  3.753E-04
  GAS

```

```

    SI2W1_S
** SI3W5_S
Calculated                      33 equilibria

Phase region boundary 21 at:  1.000E-03  3.753E-04
    GAS
    SI2W1_S
** SI3W5_S
Calculated..                    6 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 22 at:  1.000E-03  7.855E-04
    GAS
** SI2W1_S
    SI3W5_S
Calculated                      33 equilibria

Phase region boundary 23 at:  1.000E-03  7.855E-04
    GAS
** SI2W1_S
    SI3W5_S
Calculated..                    6 equilibria
Terminating at known equilibrium
Terminating at axis limit.
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex27\tcex
27.POLY3
CPU time for mapping                      4 seconds
POLY_3: @@
POLY_3: @@ Plot the diagram in the post processor
POLY_3: post

```

POLY-3 POSTPROCESSOR VERSION 3.2

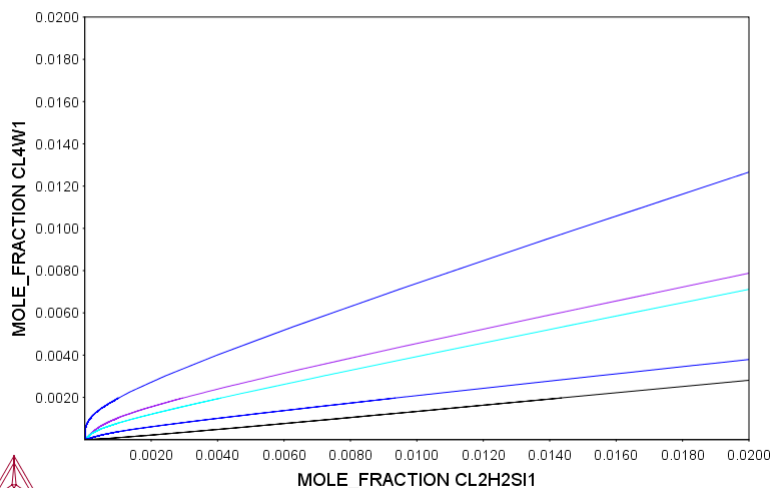
Setting automatic diagram axes

```

POST:
POST: set-title example 27a
POST: plot
... the command in full is PLOT DIAGRAM
                                example 27a

```

2016.05.16.13.59.26  
SSUB5: AR, CL4W1, CL2H2SI1, H2, CL1H1  
N=1.,X(AR)=0.9,X(CL1H1)=1.00211E-12,T=1000,P=1.01325E5



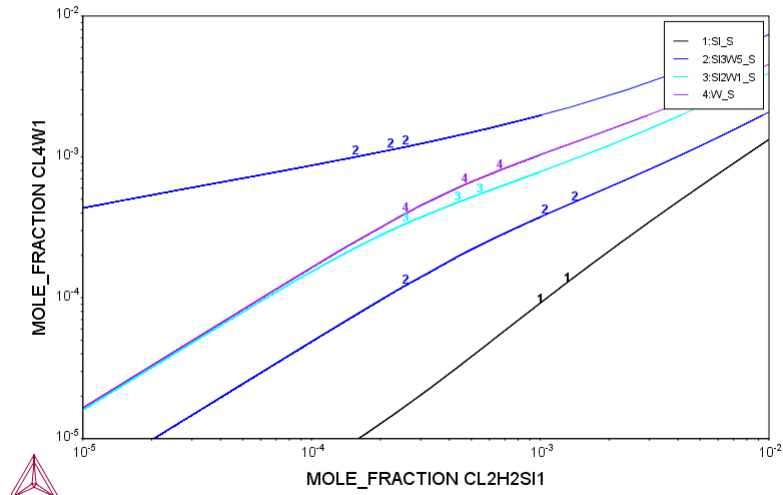
```

POST:
POST:Hit RETURN to continue
POST: @@ Better with logarithmic axis
POST: s-a-ty x log
... the command in full is SET_AXIS_TYPE
POST: s-a-ty y log
... the command in full is SET_AXIS_TYPE
POST: s-s x n 1e-5 .01
... the command in full is SET_SCALING_STATUS
POST: s-s y n 1e-5 .01
... the command in full is SET_SCALING_STATUS
POST: s-lab b
... the command in full is SET_LABEL_CURVE_OPTION
POST: @@
POST: set-title example 27b
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

# example 27b

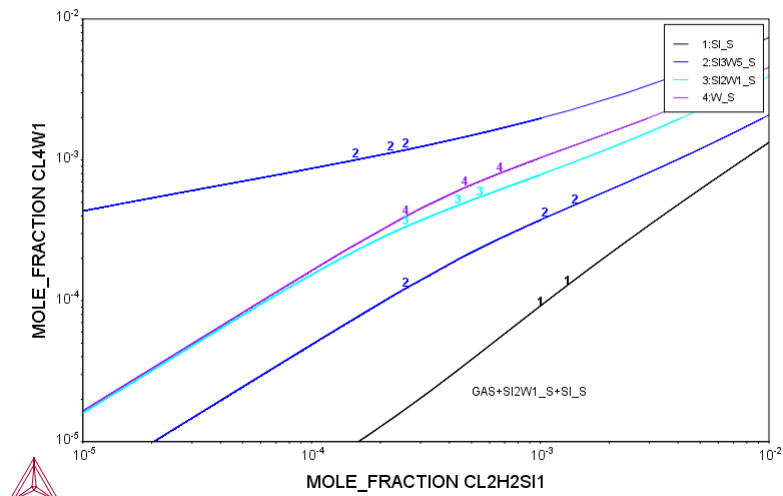
2016.05.16.13.59.26  
SSUBS: AR, CL4W1, CL2H2SI1, H2, CL1H1  
N=1., X(AR)=0.9, X(CL1H1)=1.00211E-12, T=1000, P=1.01325E5



POST:  
POST:Hit RETURN to continue  
POST: @@Identify one of the phase regions  
POST: add .0005 2e-5  
... the command in full is ADD\_LABEL\_TEXT  
Automatic phase labels? /Y/:  
Automatic labelling not always possible  
Using global minimization procedure  
Using already calculated grid  
Found the set of lowest grid points in 0 s  
Calculated POLY solution 0 s, total time 0 s  
Stable phases are: GAS+SI2W1\_S+SI\_S  
Text size: /.36/:  
POST: set-title example 27c  
POST:  
POST: plot  
... the command in full is PLOT DIAGRAM

# example 27c

2016.05.16.13.59.26  
SSUBS: AR, CL4W1, CL2H2SI1, H2, CL1H1  
N=1., X(AR)=0.9, X(CL1H1)=1.00211E-12, T=1000, P=1.01325E5



POST:  
POST: set-inter  
... the command in full is SET\_INTERACTIVE\_MODE  
POST:

## tcex28

### About

```
SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex28\tcex28.TCM" set-echo
SYS: @@
SYS: @@
SYS: @@ Example showing calculation of PRE (Pitting Resistance Equivalence)
SYS: @@ for a duplex stainless steel
SYS: @@
SYS: set-log ex28,,,,
SYS: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3: @@ set the nominal composition
POLY_3: def-mat
... the command in full is DEFINE_MATERIAL
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
L12_FCC          B2_BCC          B2_VACANCY
HIGH_SIGMA      DICTRA_FCC_A1   REJECTED
Database /TCFE8/: tcfe7
Current database: Steels/Fe-Alloys v7.0

VA DEFINED
L12_FCC          B2_BCC          B2_VACANCY
HIGH_SIGMA      DICTRA_FCC_A1   REJECTED
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/:
1st alloying element: cr 25 ni 7 mo 4 c .002 n .27 si .3 mn .3
Next alloying element:
Temperature (C) /1000/: 1050
VA DEFINED
L12_FCC          B2_BCC          B2_VACANCY
HIGH_SIGMA      DICTRA_FCC_A1   REJECTED
REINITIATING GES5 .....
... the command in full is DEFINE_ELEMENTS
FE DEFINED
... the command in full is DEFINE_ELEMENTS
CR DEFINED
... the command in full is DEFINE_ELEMENTS
NI DEFINED
... the command in full is DEFINE_ELEMENTS
MO DEFINED
... the command in full is DEFINE_ELEMENTS
C DEFINED
... the command in full is DEFINE_ELEMENTS
N DEFINED
... the command in full is DEFINE_ELEMENTS
SI DEFINED
... the command in full is DEFINE_ELEMENTS
MN DEFINED

This database has following phases for the defined system

GAS:G            LIQUID:L            BCC_A2
FCC_A1           HCP_A3            DIAMOND_FCC_A4
GRAPHITE         CEMENTITE          M23C6
M7C3            M6C              M5C2
M3C2            MC_ETA          MC_SHP
KSI_CARBIDE     A1_KAPPA          KAPPA
Z_PHASE         FE4N_LP1         FECN_CHI
PT              SIGMA          MU_PHASE
P_PHASE         R_PHASE          CHI_A12
LAVES_PHASE_C14 M3SI             G_PHASE
CR3SI           FE2SI             MSI
M5SI3           NBNI3            NI3TI
AL4C3           FE8SI2C          SIC
SI3N4           MN6N4            MN6N5

Reject phase(s) /NONE/: *
GAS:G            LIQUID:L            BCC_A2
FCC_A1           HCP_A3            DIAMOND_FCC_A4
GRAPHITE         CEMENTITE          M23C6
M7C3            M6C              M5C2
M3C2            MC_ETA          MC_SHP
KSI_CARBIDE     A1_KAPPA          KAPPA
Z_PHASE         FE4N_LP1         FECN_CHI
PT              SIGMA          MU_PHASE
P_PHASE         R_PHASE          CHI_A12
LAVES_PHASE_C14 M3SI             G_PHASE
CR3SI           FE2SI             MSI
M5SI3           NBNI3            NI3TI
AL4C3           FE8SI2C          SIC
SI3N4           MN6N4            MN6N5
REJECTED
Restore phase(s):: fcc_a1 bcc_a2 hcp_a3 m23 sigma
FCC_A1           BCC_A2            HCP_A3
M23C6           SIGMA          RESTORED
Restore phase(s): /NONE/:

.....

The following phases are retained in this system:

BCC_A2           FCC_A1            HCP_A3
M23C6           SIGMA

.....

OK? /Y/:
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ...
```

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 -OK-  
**Should any phase have a miscibility gap check? /N/: N**  
 Using global minimization procedure  
 Calculated 6136 grid points in 1 s  
 Found the set of lowest grid points in 0 s  
 Creating a new composition set SIGMA#2  
 Calculated POLY solution 0 s, total time 1 s  
**POLY\_3:**  
**POLY\_3:**  
**POLY\_3:** save tcex28 y  
 ... the command in full is SAVE\_WORKSPACES  
**POLY\_3:** l-e  
 ... the command in full is LIST\_EQUILIBRIUM  
**OUTPUT TO SCREEN OR FILE /SCREEN/:**  
**Options /VWCS/:** VWCS  
 Output from POLY-3, equilibrium = 1, label A0 , database: TCFE7  
 Conditions:  
 T=1323.15, W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(N)=2.7E-3,  
 W(SI)=3E-3, W(MN)=3E-3, P=1E5, N=1  
 DEGREES OF FREEDOM 0  
 Temperature 1323.15 K ( 1050.00 C), Pressure 1.000000E+05  
 Number of moles of components 1.00000E+00, Mass in grams 5.53180E+01



Total Gibbs energy -7.36372E+04, Enthalpy 3.91632E+04, Volume 7.43499E-06

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
C	9.2112E-05	2.0000E-05	2.8934E-05	-1.1497E+05	SER
CR	2.6597E-01	2.5000E-01	2.5102E-03	-6.5869E+04	SER
FE	6.2530E-01	6.3128E-01	1.6011E-03	-7.0817E+04	SER
MN	3.0208E-03	3.0000E-03	2.6138E-06	-1.4142E+05	SER
MO	2.3064E-02	4.0000E-02	6.3441E-04	-8.1001E+04	SER
N	1.0663E-02	2.7000E-03	4.5323E-07	-1.6070E+05	SER
NI	6.5978E-02	7.0000E-02	1.2113E-04	-9.9217E+04	SER
SI	5.9088E-03	3.0000E-03	3.2519E-09	-2.1501E+05	SER

FCC\_A1 Status ENTERED Driving force 0.0000E+00  
Moles 5.5763E-01, Mass 3.0640E+01, Volume fraction 5.5307E-01 Mass fractions:  
FE 6.36999E-01 NI 8.57940E-02 N 4.60149E-03 SI 2.58552E-03  
CR 2.34729E-01 MO 3.18218E-02 MN 3.43771E-03 C 3.18713E-05

BCC\_A2 Status ENTERED Driving force 0.0000E+00  
Moles 4.4237E-01, Mass 2.4678E+01, Volume fraction 4.4693E-01 Mass fractions:  
FE 6.24180E-01 NI 5.03909E-02 SI 3.51459E-03 N 3.39204E-04  
CR 2.68960E-01 MO 5.01537E-02 MN 2.45656E-03 C 5.26115E-06

POLY\_3:

POLY\_3:Hit RETURN to continue

POLY\_3: @@ Calculate the temperature for equal amount

POLY\_3: c-s p bcc\_a2=fix .5

... the command in full is CHANGE\_STATUS

POLY\_3: s-c t=none

... the command in full is SET\_CONDITION

POLY\_3: c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Normal POLY minimization, not global

Testing POLY result by global minimization procedure

Calculated 6136 grid points in 1 s

27 ITS, CPU TIME USED 1 SECONDS

POLY\_3: sh t

... the command in full is SHOW\_VALUE

T=1381.4276

POLY\_3: l-e,,,,

... the command in full is LIST\_EQUILIBRIUM

Output from POLY-3, equilibrium = 1, label A0 , database: TCFE7

Conditions:

W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(N)=2.7E-3, W(SI)=3E-3,

W(MN)=3E-3, P=1E5, N=1

FIXED PHASES

BCC\_A2=.5

DEGREES OF FREEDOM 0

Temperature 1381.43 K ( 1108.28 C), Pressure 1.000000E+05

Number of moles of components 1.00000E+00, Mass in grams 5.53180E+01

Total Gibbs energy -7.86534E+04, Enthalpy 4.13847E+04, Volume 7.46323E-06

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
C	9.2112E-05	2.0000E-05	2.7951E-05	-1.2043E+05	SER
CR	2.6597E-01	2.5000E-01	2.0954E-03	-7.0845E+04	SER
FE	6.2530E-01	6.3128E-01	1.3658E-03	-7.5761E+04	SER
MN	3.0208E-03	3.0000E-03	2.3755E-06	-1.4875E+05	SER
MO	2.3064E-02	4.0000E-02	4.7945E-04	-8.7785E+04	SER
N	1.0663E-02	2.7000E-03	6.6471E-07	-1.6337E+05	SER
NI	6.5978E-02	7.0000E-02	1.0967E-04	-1.0473E+05	SER
SI	5.9088E-03	3.0000E-03	4.7824E-09	-2.2005E+05	SER

BCC\_A2 Status FIXED Driving force 0.0000E+00  
Moles 5.0095E-01, Mass 2.7933E+01, Volume fraction 5.0554E-01 Mass fractions:  
FE 6.26660E-01 NI 5.38048E-02 SI 3.46210E-03 N 4.70180E-04  
CR 2.64435E-01 MO 4.86102E-02 MN 2.55179E-03 C 5.96269E-06

FCC\_A1 Status ENTERED Driving force 0.0000E+00  
Moles 4.9905E-01, Mass 2.7385E+01, Volume fraction 4.9446E-01 Mass fractions:  
FE 6.35993E-01 NI 8.65195E-02 N 4.97447E-03 SI 2.52865E-03  
CR 2.35276E-01 MO 3.12173E-02 MN 3.45719E-03 C 3.43184E-05

POLY\_3: @@ enter the PRE functions

POLY\_3: ent fun prefcc

... the command in full is ENTER\_SYMBOL

Function: 100\*w(fcc\_a1,cr)+300\*w(fcc\_a1,mo)+1600\*w(fcc\_a1,n);

POLY\_3: ent fun prebcc

... the command in full is ENTER\_SYMBOL

Function: 100\*w(bcc\_a2,cr)+300\*w(bcc\_a2,mo)+1600\*w(bcc\_a2,n);

POLY\_3: l-sy

... the command in full is LIST\_SYMBOLS

DEFINED FUNCTIONS AND VARIABLES%

PREFCC=100\*W(FCC\_A1,CR)+300\*W(FCC\_A1,MO)+1600\*W(FCC\_A1,N)

PREBCC=100\*W(BCC\_A2,CR)+300\*W(BCC\_A2,MO)+1600\*W(BCC\_A2,N)

POLY\_3: eval

... the command in full is EVALUATE\_FUNCTIONS

Name(s): \*

PREFCC=40.851953

PREBCC=41.778859

POLY\_3:Hit RETURN to continue

POLY\_3: @@ Now vary the nitrogen content

POLY\_3: s-a-v 1

... the command in full is SET\_AXIS\_VARIABLE

Condition /NONE/: w(n)

Min value /0/: .001

Max value /1/: .005

Increment /1E-04/: 1E-04

POLY\_3: li-ax

... the command in full is LIST\_AXIS\_VARIABLE

Axis No 1: W(N) Min: 1E-3 Max: 5E-3 Inc: 1E-4

POLY\_3: save tcex28 y

... the command in full is SAVE\_WORKSPACES

POLY\_3: step

... the command in full is STEP\_WITH\_OPTIONS

Option? /NORMAL/: NORMAL

No initial equilibrium, using default

Step will start from axis value 0.270000E-02

...OK

Phase Region from 0.270000E-02 for:

BCC\_A2

FCC\_A1

Global test at 3.50000E-03 .... OK

Global test at 4.50000E-03 .... OK

Global test at 4.80000E-03 .... OK

```

Terminating at 0.500000E-02
Calculated 26 equilibria

Phase Region from 0.270000E-02 for:
  BCC_A2
  FCC_A1
Global check of adding phase at 1.99041E-03
Calculated 10 equilibria

Phase Region from 0.199041E-02 for:
  BCC_A2
  FCC_A1
  SIGMA
Global test at 1.20000E-03 .... OK
Terminating at 0.100000E-02
Calculated 13 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex28\tcex
28.POLY3
POLY_3: post

```

POLY-3 POSTPROCESSOR VERSION 3.2

```

POST:
POST: @@ first plot how the temperature varies
POST: s-d-a x w(n)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t-c
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 28a
POST: plot
... the command in full is PLOT DIAGRAM

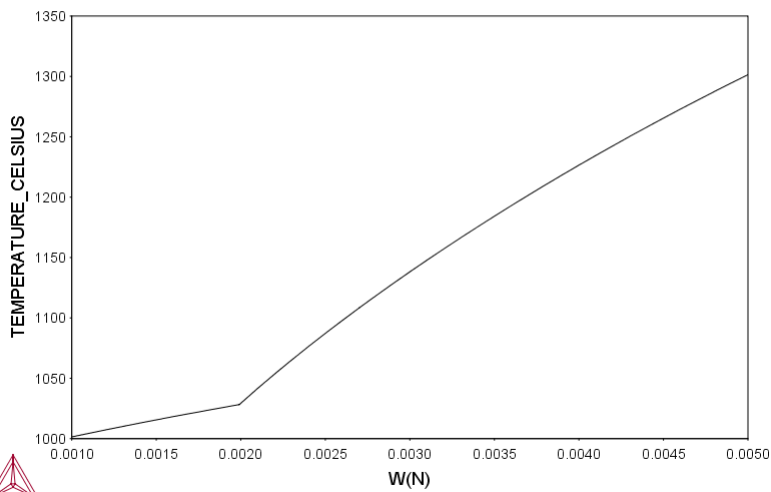
```

**example 28a**

```

2016.05.16.14.01.44
TCFE7: C, CR, FE, MN, MO, N, NI, SI
W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(SI)=3E-3, W(MN)=3E-3, P=1E5, N=1

```



```

POST:
POST: Hit RETURN to continue
POST: @@ then plot the PRE
POST: ent tab pp
... the command in full is ENTER_SYMBOL
Variable(s): prefcc prebcc
&
POST:
POST: s-d-a y pp
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: s-lab d
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 28b
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

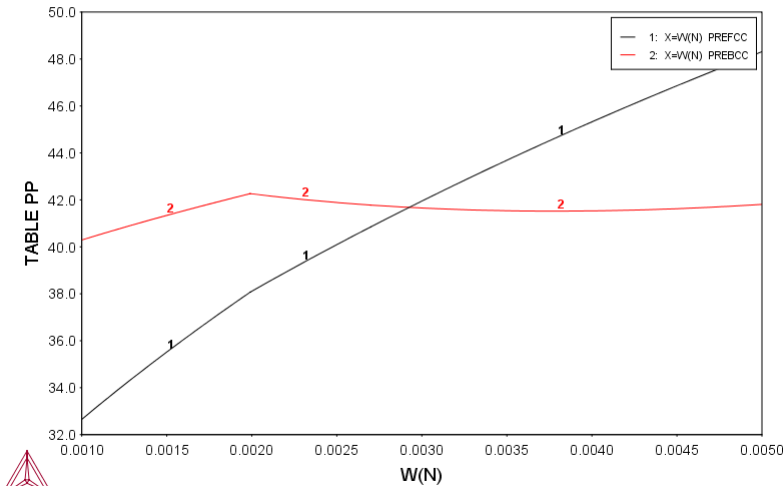
```

# example 28b

2016.05.16.14.01.44

TCFE7: C, CR, FE, MN, MO, N, NI, SI

W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(SI)=3E-3, W(MN)=3E-3, P=1E5, N=1



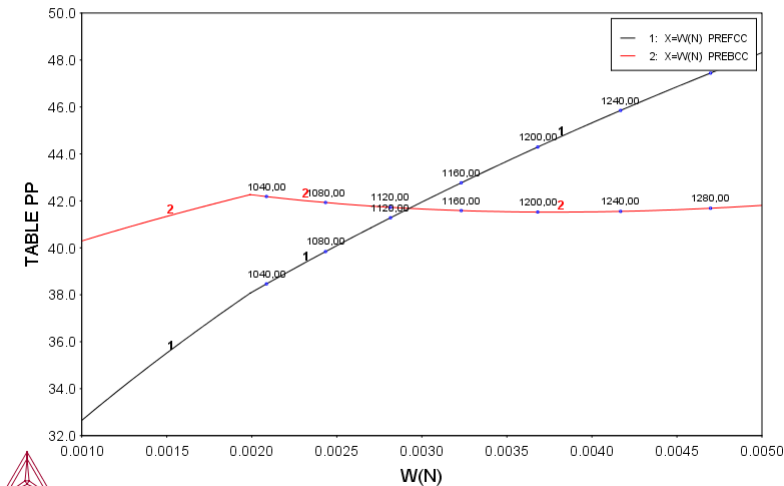
POST:  
 POST:Hit RETURN to continue  
 POST: @@ add the temperature as tic marks  
 POST: s-d-a z t-c  
 ... the command in full is SET\_DIAGRAM\_AXIS  
 POST: s-s z n 800 1300  
 ... the command in full is SET\_SCALING\_STATUS  
 POST: set-title example 28c  
 POST:  
 POST: plot  
 ... the command in full is PLOT DIAGRAM

# example 28c

2016.05.16.14.01.45

TCFE7: C, CR, FE, MN, MO, N, NI, SI

W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(SI)=3E-3, W(MN)=3E-3, P=1E5, N=1



POST:  
 POST:Hit RETURN to continue  
 POST: back  
 POLY\_3: @@ check how close we are to form Cr2N  
 POLY\_3: read tcex28  
 ... the command in full is READ\_WORKSPACES  
 POLY\_3:  
 POLY\_3: @@ Restore BCC as entered  
 POLY\_3: c-s p bcc\_a2=ent 1  
 ... the command in full is CHANGE\_STATUS  
 POLY\_3: s-c t=1323  
 ... the command in full is SET\_CONDITION  
 POLY\_3: c-e  
 ... the command in full is COMPUTE\_EQUILIBRIUM  
 Using global minimization procedure  
 Calculated 6136 grid points in 0 s  
 Found the set of lowest grid points in 0 s  
 Calculated POLY solution 0 s, total time 0 s  
 POLY\_3: l-e,,,,  
 ... the command in full is LIST\_EQUILIBRIUM  
 Output from POLY-3, equilibrium = 1, label A0 , database: TCFE7

Conditions:

T=1323, W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(N)=2.7E-3,  
 W(SI)=3E-3, W(MN)=3E-3, P=1E5, N=1

DEGREES OF FREEDOM 0

Temperature 1323.00 K ( 1049.85 C), Pressure 1.000000E+05  
 Number of moles of components 1.00000E+00, Mass in grams 5.53180E+01  
 Total Gibbs energy -7.36244E+04, Enthalpy 3.91576E+04, Volume 7.43492E-06

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
C	9.2112E-05	2.0000E-05	2.8937E-05	-1.1496E+05	SER
CR	2.6597E-01	2.5000E-01	2.5114E-03	-6.5857E+04	SER
FE	6.2530E-01	6.3128E-01	1.6017E-03	-7.0804E+04	SER
MN	3.0208E-03	3.0000E-03	2.6144E-06	-1.4140E+05	SER
MO	2.3064E-02	4.0000E-02	6.3488E-04	-8.0984E+04	SER

```

N          1.0663E-02  2.7000E-03  4.5278E-07  -1.6069E+05  SER
NI         6.5978E-02  7.0000E-02  1.2117E-04  -9.9203E+04  SER
SI         5.9088E-03  3.0000E-03  3.2485E-09  -2.1500E+05  SER

FCC A1          Status ENTERED      Driving force  0.0000E+00
Moles 5.5777E-01, Mass 3.0647E+01, Volume fraction 5.5321E-01 Mass fractions:
FE  6.37001E-01  NI  8.57922E-02  N   4.60067E-03  SI  2.58565E-03
CR  2.34728E-01  MO  3.18233E-02  MN  3.43767E-03  C   3.18660E-05

BCC A2          Status ENTERED      Driving force  0.0000E+00
Moles 4.4223E-01, Mass 2.4671E+01, Volume fraction 4.4679E-01 Mass fractions:
FE  6.24173E-01  NI  5.03822E-02  SI  3.51472E-03  N   3.38915E-04
CR  2.68972E-01  MO  5.01574E-02  MN  2.45631E-03  C   5.25959E-06
POLY_3:Hit RETURN to continue
POLY_3: @@ Find out at which temperature sigma will form
POLY_3: c-t
... the command in full is COMPUTE_TRANSITION
This command is a combination of CHANGE_STATUS and SET_CONDITION
to calculate directly when a phase may form by releasing one condition.
Phase to form: sigma
You must release one of these conditions
T=1323, W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(N)=2.7E-3,
W(SI)=3E-3, W(MN)=3E-3, P=1E5, N=1 DEGREES OF FREEDOM 0
Give the state variable to be removed /T/: t
Testing POLY result by global minimization procedure
Calculated      6136 grid points in      1 s
To form SIGMA the condition is set to T=1305.72281563
POLY_3:Hit RETURN to continue
POLY_3: @@ Find temperature for Cr2N, set start constitution first to
POLY_3: @@ make sure hcp#2 is nitride
POLY_3: s-s-c hcp_a3#2 *
... the command in full is SET_START_CONSTITUTION
POLY_3: c-t
... the command in full is COMPUTE_TRANSITION
This command is a combination of CHANGE_STATUS and SET_CONDITION
to calculate directly when a phase may form by releasing one condition.
Phase to form: hcp_a3#2
You must release one of these conditions
T=1305.72, W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(N)=2.7E-3,
W(SI)=3E-3, W(MN)=3E-3, P=1E5, N=1 DEGREES OF FREEDOM 0
Give the state variable to be removed /T/: t
Testing POLY result by global minimization procedure
Calculated      6136 grid points in      0 s
To form HCP_A3 the condition is set to T=1254.68882961
POLY_3: l-e,,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium =      1, label A0 , database: TCFe7

Conditions:
T=1254.69, W(CR)=0.25, W(NI)=7E-2, W(MO)=4E-2, W(C)=2E-5, W(N)=2.7E-3,
W(SI)=3E-3, W(MN)=3E-3, P=1E5, N=1
DEGREES OF FREEDOM 0

Temperature 1254.69 K ( 981.54 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 5.53180E+01
Total Gibbs energy -6.78789E+04, Enthalpy 3.60849E+04, Volume 7.36619E-06

Component      Moles      W-Fraction  Activity  Potential  Ref.stat
C              9.2112E-05  2.0000E-05  2.9898E-05  -1.0868E+05  SER
CR             2.6597E-01  2.5000E-01  3.1144E-03  -6.0211E+04  SER
FE             6.2530E-01  6.3128E-01  1.9691E-03  -6.4994E+04  SER
MN             3.0208E-03  3.0000E-03  2.9050E-06  -1.3300E+05  SER
MO             2.3064E-02  4.0000E-02  6.9498E-04  -7.5859E+04  SER
N              1.0663E-02  2.7000E-03  2.7031E-07  -1.5777E+05  SER
NI             6.5978E-02  7.0000E-02  1.3051E-04  -9.3306E+04  SER
SI             5.9088E-03  3.0000E-03  2.3872E-09  -2.0711E+05  SER

FCC A1          Status ENTERED      Driving force  0.0000E+00
Moles 7.2826E-01, Mass 3.9978E+01, Volume fraction 7.2581E-01 Mass fractions:
FE  6.52952E-01  NI  8.17394E-02  N   3.69563E-03  SI  3.36288E-03
CR  2.30278E-01  MO  2.45688E-02  MN  3.37715E-03  C   2.69108E-05

SIGMA          Status ENTERED      Driving force  0.0000E+00
Moles 1.4476E-01, Mass 8.2984E+00, Volume fraction 1.4547E-01 Mass fractions:
FE  5.25243E-01  MO  1.15108E-01  MN  1.74847E-03  C   0.00000E+00
CR  3.22933E-01  NI  3.48841E-02  SI  8.39239E-05  N   0.00000E+00

BCC A2          Status ENTERED      Driving force  0.0000E+00
Moles 1.2697E-01, Mass 7.0417E+00, Volume fraction 1.2872E-01 Mass fractions:
FE  6.33206E-01  NI  4.47345E-02  SI  4.37633E-03  N   2.29340E-04
CR  2.76020E-01  MO  3.90957E-02  MN  2.33369E-03  C   4.33440E-06

HCP_A3#2        Status ENTERED      Driving force  0.0000E+00
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:
CR  8.23740E-01  MO  3.89056E-02  NI  1.31664E-03  C   2.52562E-04
N   1.08069E-01  FE  2.70648E-02  MN  6.51302E-04  SI  2.27285E-08
POLY_3: @@ Rapid cooling needed to avoid these phases!
POLY_3: set-inter
... the command in full is SET_INTERACTIVE
POLY_3:

```

**About**

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software (build 9533) running on WinNT 64-bit wordlength  
Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118  
License library version: 8.5.1.0017  
Linked: Mon May 16 09:31:44 2016

```
SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex29\tcex29.TCM"SYS: set-echo
```

```
SYS: @@
```

```
SYS: @@
```

```
SYS: @@ Calculation of speciation of a gas
```

```
SYS: @@
```

```
SYS: set-log ex29,,,,
```

```
SYS: go da
```

```
... the command in full is GOTO_MODULE
```

```
THERMODYNAMIC DATABASE module
```

```
Current database: Steels/Fe-Alloys v8.0
```

```
VA DEFINED
```

```
L12 FCC
```

```
B2_BCC
```

```
B2_VACANCY
```

```
HIGH SIGMA
```

```
DICTRA_FCC_A1 REJECTED
```

```
TDB_TCFE8: sw ssu5
```

```
... the command in full is SWITCH_DATABASE
```

```
Current database: SGTE Substances Database v5.1
```

```
VA DEFINED
```

```
TDB_SSUB5:
```

```
TDB_SSUB5: d-sys c o h s
```

```
... the command in full is DEFINE_SYSTEM
```

```
C O H
```

```
S DEFINED
```

```
TDB_SSUB5: l-sys
```

```
... the command in full is LIST_SYSTEM
```

```
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/: CONSTITUENT
```

```
GAS:G :C C1H1 C1H1O1 C1H1O2 C1H2 C1H2O1 C1H2O2_CIS C1H2O2_DIOXIRANE
C1H2O2_TRANS C1H3 C1H3O1 CH2OH C1H3O1_CH3O C1H4 C1H4O1 C1H4S1 C1O1 C1O1S1
C1O2 C1S1 C1S2 C2 C2H1 C2H2 C2H2O1 C2H3 C2H4 C2H4O1 ACETALDEHYDE
C2H4O1_OXIRANE C2H4O2 ACETICACID C2H4O2_DIOXETANE C2H4O3 123TRIOXOLANE
C2H4O3_124TRIOXOLANE C2H5 C2H6 C2H6O1 C2H6O2 C2O1 C3 C3H1 C3H4_1 C3H4_2
C3H6_1 C3H6_2 C3H6O1 C3H8 C3O2 C4 C4H1 C4H1O_1 C4H1O_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 C6O C6H6 C6H6O1 H H2 H1O1 H1O2 H2O1 H2O2 H1S1 H2S1
H2S2 H1O1S1_HSO H1O1S1_SOH H2O1S1_H2SO H2O1S1_HSOH H2O4S1 O O2 O3 O1S1
O1S2 O2S1 O3S1 S S2 S3 S4 S5 S6 S7 S8:
```

```
GRAPHITE :C:
```

```
GRAPHITE_L :C:
```

```
DIAMOND :C:
```

```
C1H2O2_L :C1H2O2:
```

```
C1H2S3_L :C1H2S3:
```

```
C1H4O1_L :C1H4O1:
```

```
C1H4S1_L :C1H4S1:
```

```
C1S2_L :C1S2:
```

```
C2H4O2_L :C2H4O2:
```

```
C2H6O1_L :C2H6O1:
```

```
C2H6O2_L :C2H6O2:
```

```
C6O_S :C6O:
```

```
C6H6_L :C6H6:
```

```
H2O1_L :H2O1:
```

```
H2O2_L :H2O2:
```

```
H2S1_L :H2S1:
```

```
H2S2_L :H2S2:
```

```
H2O4S1_L :H2O4S1:
```

```
H4O5S1_L :H4O5S1:
```

```
H6O6S1_L :H6O6S1:
```

```
H10O8S1_L :H10O8S1:
```

```
H15O10_5S1_L :H15O10.5S1:
```

```
H8O7S1_L :H8O7S1:
```

```
O3S1_L :O3S1:
```

```
S_S :S:
```

```
S_S2 :S:
```

```
S_L :S:
```

```
TDB_SSUB5:Hit RETURN to continue
```

```
TDB_SSUB5: get
```

```
... the command in full is GET_DATA
```

```
REINITIATING GES5 .....
```

```
ELEMENTS .....
```

```
SPECIES .....
```

```
PHASES .....
```

```
PARAMETERS ...
```

```
FUNCTIONS ....
```

List of references for assessed data

```
C1<G> T.C.R.A.S. Class: 1
```

```
C1<G> C<G>
```

```
C1H1<G> T.C.R.A.S. Class: 2
```

```
C1H1<G> CH<G>
```

```
C1H1O1<G> T.C.R.A.S. Class: 4
```

```
C1H1O1<G> HCO<G>
```

```
FORMYL <GAS>
```

```
C1H1O2<G> T.C.R.A.S. Class: 6
```

```
C1H1O2<G>
```

```
C1H2<G> T.C.R.A.S. Class: 5
```

```
C1H2<G> CH2<G> METHYLENE
```

```
METHYLENE <GAS>
```

```
C1H2O1<G> T.C.R.A.S. Class: 5
```

```
C1H2O1<G> CH2O<G>
```

```
FORMALDEHYDE <GAS>
```

```
C1H2O2_CIS<G> T.C.R.A.S. Class: 5
```

```
C1H2O2_CIS<G>
```

```
C1H2O2_DIOXIRANE<G> T.C.R.A.S. Class: 6
```

```
C1H2O2_DIOXIRANE<G>
```

```
S298 corrected and cp refitted
```

```
due to corrected data in IVTAN2000 7/2002
```

```
C1H2O2_TRANS<G> T.C.R.A.S. Class: 5
```

```
C1H2O2_TRANS<G>
```

C1H3<G> T.C.R.A.S. Class: 5  
 C1H3<G> CH3<G>  
 METHYL, Gaseous Standard State.  
 C1H3O1\_CH2OH<G> T.C.R.A.S. Class: 6  
 C1H3O1\_CH2OH<G>  
 C1H3O1\_CH3O<G> T.C.R.A.S. Class: 5  
 C1H3O1\_CH3O<G>  
 C1H4<G> T.C.R.A.S. Class: 5  
 C1H4<G> CH4<G> METHANE  
 METHANE, Gaseous Standard State.  
 C1H4O1<G> T.C.R.A.S. Class: 5  
 C1H4O1<G> CH3OH<G>  
 METHANOL <GAS>  
 C1H4S1<G> THERMODATA 04/98 TC  
 C1H4S1<G> METHANETHIOL.  
 C1O1<G> JANAF THERMOCHEMICAL TABLES SGTE \*\*  
 C1O1<G> CO<G>  
 CARBON MONOXIDE <GAS>  
 STANDARD STATE : CODATA KEY VALUE. /CP FROM JANAF PUB. 9/65  
 C1O1S1<G> T.C.R.A.S. Class: 2  
 C1O1S1<G> COS<G>  
 CARBON OXIDE SULFIDE <GAS>  
 C1O2<G> T.C.R.A.S. Class: 2  
 C1O2<G> CO2<G>  
 CARBON DIOXIDE <GAS>  
 C1S1<G> T.C.R.A.S. Class: 1  
 C1S1<G> CS<G>  
 CARBON MONOSULFIDE <GAS>  
 C1S2<G> T.C.R.A.S. Class: 3  
 C1S2<G> CS2<G>  
 CARBON DISULFIDE <GAS>  
 C2<G> T.C.R.A.S. Class: 2  
 C2<G>  
 CARBON Diatomic Gas.  
 C2H1<G> T.C.R.A.S. Class: 6  
 C2H1<G> C2H<G>  
 CCH RADICAL <GAS>  
 C2H2<G> T.C.R.A.S. Class: 2  
 C2H2<G>  
 ACETYLENE (ETYLENE). Gaseous Standard State.  
 C2H2O1<G> T.C.R.A.S. Class: 6  
 C2H2O1<G>  
 OXIRENE  
 S298 corrected and cp refitted  
 due to corrected data in IVTAN2000 7/2002  
 C2H3<G> T.C.R.A.S. Class: 6  
 C2H3<G>  
 DICARBON TRIHYDRIDE, Gaseous Standard State.  
 C2H4<G> T.C.R.A.S. Class: 6  
 C2H4<G>  
 ETHYLENE. Gaseous Standard State.  
 C2H4O1\_ACETALDEHYDE<G> T.C.R.A.S. Class: 5  
 C2H4O1\_ACETALDEHYDE<G>  
 C2H4O1\_OXIRANE<G> T.C.R.A.S. Class: 6  
 C2H4O1\_OXIRANE<G>  
 S298 corrected and cp refitted  
 due to corrected data in IVTAN2000 7/2002  
 C2H4O2\_ACETICACID<G> T.C.R.A.S. Class: 5  
 C2H4O2\_ACETICACID<G>  
 C2H4O2\_DIOXETANE<G> T.C.R.A.S. Class: 6  
 C2H4O2\_DIOXETANE<G>  
 S298 corrected and cp refitted  
 due to corrected data in IVTAN2000 7/2002  
 typing error corrected 12/06  
 C2H4O3\_123TRIOXOLANE<G> T.C.R.A.S. Class: 7  
 C2H4O3\_123TRIOXOLANE<G>  
 S298 corrected and cp refitted  
 due to corrected data in IVTAN2000 7/2002  
 C2H4O3\_124TRIOXOLANE<G> T.C.R.A.S. Class: 7  
 C2H4O3\_124TRIOXOLANE<G>  
 S298 corrected and cp refitted  
 due to corrected data in IVTAN2000 7/2002  
 typing error corrected 12/06  
 C2H5<G> T.C.R.A.S. Class: 6  
 C2H5<G>  
 ETHYL radical. Gaseous Standard State.  
 C2H6<G> T.C.R.A.S. Class: 6  
 C2H6<G>  
 ETHANE. Gaseous Standard State.  
 C2H6O1<G> T.C.R.A.S. Class: 6  
 C2H6O1<G> C2H6O<G>  
 ETHANOL <GAS>  
 C2H6O2<G> THERMODATA  
 C2H6O2<G>  
 E-GLYCOL <GAS>.Data revised by THDA.  
 C2O1<G> T.C.R.A.S. Class: 5  
 C2O1<G> C2O<G>  
 C3<G> T.C.R.A.S. Class: 6  
 C3<G>  
 CARBON <TRIATOMIC GAS>  
 C3H1<G> T.C.R.A.S. Class: 6  
 C3H1<G> C3H<G>  
 2-PROPYNYLIDYNE (gaseous state)  
 S298 corrected and cp refitted  
 due to corrected data in IVTAN2000 7/2002  
 C3H4\_1<G> STULL WESTRUM SINKE 1969 SGTE  
 C3H4\_1<G>  
 ALLENE = 1,2-PROPADIENE (gaseous state)  
 EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.  
 C3H4\_2<G> STULL WESTRUM SINKE 1969 SGTE  
 C3H4\_2<G>  
 PROPYNE (METHYLACETYLENE) (gaseous state)  
 EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.  
 C3H6O1<G> THERMODATA 01/93  
 C3H6O1<G> ACETONE gas  
 ACETONE (gaseous state)  
 28/01/93  
 C3H6\_1<G> T.C.R.A.S. Class: 6 4.09.85  
 C3H6\_1<G> Cyclopropane gas  
 C3H6\_2<G> STULL WESTRUM SINKE 1969 SGTE  
 C3H6\_2<G> PROPENE gas  
 PROPENE (gaseous state)  
 EXTRAPOLATION BY THERMODATA FROM 1000 TO 1350K.  
 C3H8<G> THERMODATA SGTE  
 C3H8<G> PROPANE gas  
 PROPANE <Gaseous Standard State>

C302<G> T.C.R.A.S. Class: 6  
 C302<G>  
 C4<G> T.C.R.A.S. Class: 7  
 C4<G>  
 C4H1<G> T.C.R.A.S. Class: 6  
 C4H1<G> C4H<G> 1,3-BUTADIENYL gas  
 1,3-BUTADIENYL (Gaseous Standard State).  
 Data provided by T.C.R.A.S. in 2000  
 C4H10\_1<G> T.C.R.A.S. Class: 4  
 C4H10\_1<G> BUTANE gas  
 BUTANE (Gaseous Standard State).  
 Data provided by T.C.R.A.S. in 2000  
 C4H10\_2<G> T.C.R.A.S. Class: 4  
 C4H10\_2<G> METHYLPROPANE N-BUTANE gas  
 METHYLPROPANE N-BUTANE (Gaseous Standard State).  
 Data provided by T.C.R.A.S. in 2000  
 C4H2\_1<G> THERMODYNAMIC DATA 1978 ST  
 C4H2\_1<G> 1,3-BUTADIENE gas  
 C4H2\_2<G> THERMODYNAMIC DATA 06/93 ST  
 C4H2\_2<G> BUTADIENE (BIACETYLENE) gas  
 C4H4\_1<G> T.C.R.A.S. Class: 6  
 C4H4\_1<G> 1,3-CYCLOBUTADIENE gas.  
 1,3-CYCLOBUTADIENE. Gaseous Standard State.  
 Data provided by T.C.R.A.S. in 2000  
 C4H4\_2<G> STULL WESTRUM SINKE 1969 SGTE  
 C4H4\_2<G> 1-BUTEN-3-YNE VINYLACETYLENE gas  
 1-BUTEN-3-YNE VINYLACETYLENE. Gaseous Standard State.  
 EXTRAPOLATION BY THERMODYNAMIC DATA FROM 1000 TO 1350K.  
 C4H6\_1<G> STULL WESTRUM SINKE 1969 SGTE  
 C4H6\_1<G>  
 1,2-BUTADIENE  
 EXTRAPOLATION BY THERMODYNAMIC DATA FROM 1000 TO 1350K.  
 C4H6\_2<G> STULL WESTRUM SINKE 1969 SGTE  
 C4H6\_2<G>  
 1,3-BUTADIENE  
 EXTRAPOLATION BY THERMODYNAMIC DATA FROM 1000 TO 1350K.  
 C4H6\_3<G> STULL WESTRUM SINKE 1969 SGTE  
 C4H6\_3<G>  
 1-BUTYNE ETHYLACETYLENE  
 EXTRAPOLATION BY THERMODYNAMIC DATA FROM 1000 TO 1350K.  
 C4H6\_4<G> STULL WESTRUM SINKE 1969 SGTE  
 C4H6\_4<G>  
 2-BUTYNE DIMETHYLACETYLENE  
 EXTRAPOLATION BY THERMODYNAMIC DATA 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> THERMODYNAMIC DATA 04/98 TC  
 C4H8\_1<G> 1-BUTENE gas  
 C4H8\_2<G> THERMODYNAMIC DATA 04/98 TC  
 C4H8\_2<G> (E)-2-BUTENE gas  
 C4H8\_3<G> THERMODYNAMIC DATA 04/98 TC  
 C4H8\_3<G> (Z)-2-BUTENE gas  
 C4H8\_4<G> THERMODYNAMIC DATA 04/98 TC  
 C4H8\_4<G> CYCLOBUTANE gas  
 C4H8\_5<G> THERMODYNAMIC DATA 04/98 TC  
 C4H8\_5<G> 2-METHYLPROPENE gas  
 C4H8\_6<G> THERMODYNAMIC DATA 04/98 TC  
 C4H8\_6<G> METHYL CYCLOPROPANE gas  
 C5<G> T.C.R.A.S. Class: 7  
 C5<G>  
 C60<G> MHR-95  
 C60<G>  
 Data processed from [94Kor/Sid] M.V. Korobov, L.N. Sidorov,  
 J. Chem. Thermo, 26, 61-73 (1994). Recalculated from the rotational  
 data in [91McK] and vibration frequencies in [94Kor/Sid]. Note that  
 a frequency with degeneracy 5 is missing from list in [94Kor/Sid];  
 taken to be 419 cm<sup>-1</sup>, 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<sup>-1</sup> for the reaction  
 60Cg>C60g>and that given by [94Kor/Sid] in their Table 5,  
 -8950 J mol K<sup>-1</sup>. Enthalpy of formation: DfH = 2588 kJ/mol from  
 DsubH(298.15K) = 166 +/- 11 kJ mol<sup>-1</sup> [94Kor/Sid]. Vapour pressure  
 values reproduced very well.  
 [91McK] J.T. McKinnon, J. Phys. Chem. 95 8941(1993).  
 C6H6<G> T.C.R.A.S. Class: 5  
 C6H6<G> BENZENE gas  
 BENZENE (Gaseous Standard State).  
 Data provided by T.C.R.A.S. in 2000  
 C6H601<G> THERMODYNAMIC DATA 01/93  
 C6H601<G>  
 PHENOL gas  
 28/01/93  
 H1<G> JANAF 1982; ASSESSMENT DATED 3/77 SGTE \*\*  
 H1<G> H<G>  
 HYDROGEN <MONATOMIC GAS>  
 H101<G> T.C.R.A.S. Class: 1  
 H101<G> OH<G>  
 H101S1\_HSO<G> T.C.R.A.S. Class: 4  
 H101S1\_HSO<G>  
 H101S1\_SOH<G> T.C.R.A.S. Class: 5  
 H101S1\_SOH<G>  
 H102<G> T.C.R.A.S. Class: 4  
 H102<G> H2O<G>  
 H1S1<G> T.C.R.A.S. Class: 2  
 H1S1<G> HS<G>  
 H2<G> JANAF THERMOCHEMICAL TABLES SGTE \*\*  
 H2<G> H2<G>  
 HYDROGEN<G>  
 STANDARD STATE FROM CODATA KEY VALUES. CP FROM JANAF PUB. 3/61  
 H201<G> T.C.R.A.S. Class: 1  
 H201<G> H2O<G>  
 WATER <GAS>, STEAM  
 H201S1\_H2SO<G> T.C.R.A.S. Class: 4  
 H201S1\_H2SO<G>  
 H201S1\_HSOH<G> T.C.R.A.S. Class: 4  
 H201S1\_HSOH<G>  
 H202<G> JANAF SECOND EDIT SGTE  
 H202<G> H2O2<G>  
 HYDROGEN PEROXIDE <GAS>  
 H204S1<G> JANAF 1982; ASSESSMENT DATED 9/77 SGTE  
 H204S1<G> H2SO4<G>  
 SULFURIC ACID <GAS>  
 H2S1<G> T.C.R.A.S. Class: 2  
 H2S1<G> H2S<G>  
 HYDROGEN SULFIDE <GAS>

H2S2<G> K.C. MILLS SGTE \*\*  
 H2S2<G> H2S2<G>  
 DIHYDROGEN DISULFIDE <GAS>  
 O1<G> TCRAS 02/06/80  
 O1<G> O<G>  
 O1S1<G> T.C.R.A.S. Class: 3  
 O1S1<G> SO<G>  
 SULFUR MONOXIDE <GAS>  
 O1S2<G> JANAF THERMOCHEMICAL TABLES SGTE \*\*  
 O1S2<G> S2O<G>  
 DISULFUR MONOXIDE <GAS>  
 PUBLISHED BY JANAF AT 9/65  
 O2<G> TCRAS 21/06/90  
 O2<G>  
 OXYGEN Gaseous Standard State.  
 O2S1<G> JANAF THERMOCHEMICAL TABLES SGTE \*\*  
 O2S1<G> SO2<G>  
 SULFUR DIOXIDE <GAS>  
 PUBLISHED BY JANAF AT 6/61  
 O3<G> TCRAS 02/06/80  
 O3<G>  
 OZONE Gaseous Standard State.  
 O3S1<G> JANAF THERMOCHEMICAL TABLES SGTE \*\*  
 O3S1<G> SO3<G>  
 SULFUR TRIOXIDE <GAS>  
 PUBLISHED BY JANAF AT 9/65  
 S1<G> T.C.R.A.S. Class: 1  
 S1<G> S<G>  
 SULFUR <GAS>  
 S2<G> T.C.R.A.S. Class: 4  
 S2<G> S2<G>  
 SULFUR <DIATOMIC GAS>  
 S3<G> T.C.R.A.S. Class: 5  
 S3<G> S3<G>  
 SULFUR <3-ATOMIC GAS>  
 S4<G> T.C.R.A.S. Class: 6  
 S4<G> S4<G>  
 SULFUR <4-ATOMIC GAS>  
 S5<G> T.C.R.A.S. Class: 6  
 S5<G> S5<G>  
 SULFUR <5-ATOMIC GAS>  
 S6<G> T.C.R.A.S. Class: 6  
 S6<G> S6<G>  
 SULFUR <6-ATOMIC GAS>  
 S7<G> T.C.R.A.S. Class: 7  
 S7<G> S7<G>  
 SULFUR <7-ATOMIC GAS>  
 S8<G> T.C.R.A.S. Class: 7  
 S8<G> S8<G>  
 SULFUR <OCTATOMIC GAS>  
 C1H2O2<L> THERMODATA 01/93  
 C1H2O2 Liquid HCOOH Liquid  
 FORMIC ACID MONOMERIC  
 28/01/93  
 C1H2S3<L> THERMODATA 01/86 BC  
 C1H2S3 Liquid H2C1S2 Liquid  
 C1H4O1<L> I. BARIN 3rd. Edition  
 C1H4O1 Liquid CH3OH Liquid  
 METHANOL (Liquid). H298 and S298 modified.  
 C1H4S1<L> THERMODATA 04/99 HH  
 C1H4S1<L> METHANETHIOL.  
 C1S2<L> KUBASCHEWSKI EVANS ALCOCK 1967 SGTE  
 C1S2 CS2  
 CARBON DISULFIDE  
 C1S2 MELTS AT 161.15K LF=1.05(0.1)KCAL/MOLE  
 C2H4O2<L> THERMODATA 01/93  
 C2H4O2 Liquid  
 ACETIC ACID (Liquid)  
 28/01/93 Tb=389K.  
 C2H6O1<L> THERMODATA 01/93  
 C2H6O1 Liquid C2H6O Liquid  
 ETHANOL (Liquid)  
 28/01/93  
 C2H6O2<L> THERMODATA  
 C2H6O2 Liquid  
 E-GLYCOL (Liquid)  
 Data revised by THDA.  
 C60 MHR-95  
 C60  
 Data processed from [94Kor/Sid] M.V. Korobov, L.N. sidorov, J. Chem.  
 The  
 Fitted to the data in [94Kor/Sid], who took the phase transition at  
 257K  
 that [94Kor/Sid] do not give an explicit value for S(298.15K).  
 S(298.15K) = 422.6 J mol K-1 was calculated from S(300) = 425.8 and Cp  
 e  
 calculated from DrS(298) for 60C<graphite>=C60 given by [94Kor/Sid]  
 in their Table 5, which gives S(298.15K) = 425.4 J mol K-1.  
 Enthalpy of formation : DfH = +2422 +/- 14 kJ/mol from [92Ste/Chi],  
 the value preferred, if obliquely, by [94Kor/Sid].  
 [92Ste/Chi]W.V. Steele, R.D. Chirico, N.K. Smith, W.e. Billups,  
 P.R. Elmore, A.E. Wheeler, J. Phys. Chem. 96 4731 (1993).  
 C6H6<L> THERMODATA 04/99 BC  
 C6H6 Liquid BENZENE Liquid  
 C1<DIAMOND> S.G.T.E. \*\*  
 C DIAMOND  
 <DIAMOND>  
 Data from SGTE Unary DB, data added by atd 7/9/95, H298-H0 taken  
 from 1994 database (ex THERMODATA 01/93)  
 C1<GRAPHITE> S.G.T.E. \*\*  
 C GRAPHITE  
 Data from SGTE Unary DB, pressure dependent data added by atd 7/9/95  
 H1008S1<L> THERMODATA 01/93  
 H1008S1 Liquid H2SO4-4H2O Liquid  
 SULFURIC ACID TETRAHYDRATE.  
 28/01/93  
 H15010.5S1<L> THERMODATA 01/93  
 H15010.5S1 Liquid H2SO4-6.5H2O Liquid  
 SULFURIC ACID HEMIHEXAHYDRATE.  
 28/01/93  
 H2O1<L> T.C.R.A.S. Class: 4  
 H2O1 Liquid H2O Liquid Pure\_Water  
 WATER  
 T.C.R.A.S. Class: 4 cp modified by atd 12/9/94 and 5/7/2002  
 H2O2<L> THERMODATA 01/93  
 H2O2 Liquid H2O2 Liquid



```

HYDROGEN PEROXIDE
28/01/93
H2O4S1<L> THERMODATA 01/93
H2O4S1_Liquid H2SO4_Liquid
SULFURIC ACID
28/01/93 Tb = 553K.
S298 modified by NPL 24/11/94. Negative value in Thermodata.
H2S1<L> THERMODATA 12/94 KK
H2S1_Liquid H2S_Liquid
H2S2<L> THERMODATA 11/99 KK
H2S2_Liquid H2S2_Liquid
H4O5S1<L> THERMODATA 01/93
H4O5S1_Liquid H2SO4-H2O_Liquid
SULFURIC ACID MONOHYDRATE.
28/01/93
H6O6S1<L> THERMODATA 01/93
H6O6S1_Liquid H2SO4-2H2O_Liquid
H2SO4-2H2O
28/01/93
H8O7S1<L> Janaf 4th. Edition
H8O7S1_Liquid H2SO4-3H2O_Liquid
SULFURIC ACID TRIHYDRATE
O3S1<L> THERMODATA 12/94 KK
O3S1_Liquid SO3_Liquid
S1 T.C.R.A.S Class: 5
S1 S
Data provided by T.C.R.A.S. October 1994.
Data refitted by I.A.
-OK-
TDB_SSUB5: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3: l-st c
... the command in full is LIST_STATUS
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS      REF. STATE      T(K)            P(Pa)
VA              ENTERED      SER
C              ENTERED      SER
H              ENTERED      SER
O              ENTERED      SER
S              ENTERED      SER
POLY_3: s-i-a n(h2)=10
... the command in full is SET_INPUT_AMOUNTS
POLY_3: l-c
... the command in full is LIST_CONDITIONS
N(H)=20
DEGREES OF FREEDOM 5
POLY_3: s-i-a n(c1o2)=5
... the command in full is SET_INPUT_AMOUNTS
POLY_3: s-i-a n(o2s1)=0.1
... the command in full is SET_INPUT_AMOUNTS
POLY_3: l-c
... the command in full is LIST_CONDITIONS
N(H)=20, N(C)=5, N(O)=10.2, N(S)=0.1
DEGREES OF FREEDOM 2
POLY_3: s-c t=1000 p=1e5
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      125 grid points in      0 s
Found the set of lowest grid points in      0 s
Calculated POLY solution      0 s, total time      0 s
POLY_3: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
Output from POLY-3, equilibrium =      1, label A0 , database: SSUB5

Conditions:
N(H)=20, N(C)=5, N(O)=10.2, N(S)=0.1, T=1000, P=1E5
DEGREES OF FREEDOM 0

Temperature 1000.00 K ( 726.85 C), Pressure 1.000000E+05
Number of moles of components 3.53000E+01, Mass in grams 2.46609E+02
Total Gibbs energy -4.82824E+06, Enthalpy -1.54921E+06, Volume 1.23971E+00

Component      Moles      W-Fraction Activity Potential Ref.stat
C              5.0000E+00  2.4352E-01 3.4847E-02 -2.7910E+04 SER
H              2.0000E+01  8.1741E-02 1.0525E-04 -7.6154E+04 SER
O              1.0200E+01  6.6173E-01 7.2141E-17 -3.0903E+05 SER
S              1.0000E-01  1.3003E-02 9.1466E-08 -1.3476E+05 SER

GAS              Status ENTERED      Driving force 0.0000E+00
Moles 3.5300E+01, Mass 2.4661E+02, Volume fraction 1.0000E+00 Mass fractions:
O 6.61734E-01 C 2.43523E-01 H 8.17406E-02 S 1.30027E-02
Constitution:
H2      4.42736E-01 C3H6_2      1.11399E-13 C4H4_2      3.35580E-21
H2O1    2.15350E-01 H1O1S1_SOH 3.35036E-14 C4H8_6      1.82465E-21
ClO1    1.95778E-01 C2H6O1    2.98678E-14 O2      1.76901E-21
ClO2    1.36417E-01 C2H5      2.60816E-14 C2O1    1.66878E-21
H2S1    6.57218E-03 C3H8      1.55219E-14 S5      8.95084E-22
ClH4    3.01187E-03 ClH3O1_CH2OH 7.69302E-15 C2H2O1    5.16353E-22
ClO1S1  1.34465E-04 H2O1S1_H2SO 2.59570E-15 C4H6_5      3.26857E-22
H1S1    5.08063E-08 C3H6O1    1.36487E-15 C4H8_4      5.15316E-23
ClH2O1  4.89873E-08 C2H3      1.30277E-15 H2O4S1    1.59729E-23
ClH2O2_CIS 4.46604E-08 C3H4_2    1.28184E-15 C4H2_1    8.50232E-24
H2S2    3.75745E-08 C3O2      7.11139E-16 C4H2_2    8.48033E-24
ClS2    1.41821E-08 C3H4_1    3.44164E-16 C6H6O1    6.55562E-24
S2      1.10500E-08 H1O1S1_HSO 1.08974E-16 H1O2    1.72311E-24
ClH2O2_TRANS 6.42811E-09 C3H6_1    5.22179E-17 C2H1    3.18714E-25
C2H6    3.64609E-09 ClH3O1_CH3O 1.80849E-17 S6      2.65463E-26
C2H4    3.02667E-09 C2H4O1_OXIRA 2.11511E-18 ClH1    5.08634E-27
H        1.51148E-09 C4H6_2    1.29360E-18 C4H4_1    4.75003E-27
ClH4O1  1.14083E-09 S4      1.12104E-18 C3H1    9.91558E-28
O2S1    2.26895E-10 C4H8_5    6.89221E-19 ClH2O2_DIOXI 4.40433E-30
ClH3    1.88514E-10 C4H8_1    5.18832E-19 C      1.00000E-30
ClH4S1  1.76437E-10 C4H8_2    4.53214E-19 C2      1.00000E-30
H2O1S1_HSOH 8.67082E-11 C4H8_3    3.93010E-19 C2H4O2_DIOXE 1.00000E-30
C2H4O1_ACETA 2.61120E-11 C2H6O2    2.59417E-19 C2H4O3_123TR 1.00000E-30
C2H2    1.43254E-11 ClH2      2.13894E-19 C2H4O3_124TR 1.00000E-30
O1S1    1.05406E-11 C4H10_1    8.31953E-20 C3      1.00000E-30
ClH1O1  9.19785E-12 C4H10_2    4.22679E-20 C4      1.00000E-30
ClS1    5.40802E-12 C6H6      3.95182E-20 C4H1    1.00000E-30

```

```

C2H4O2_ACETI 4.53120E-12 H2O2 2.47048E-20 C5 1.00000E-30
H1O1 1.61961E-12 C4H6_4 1.91129E-20 C60 1.00000E-30
O1S2 9.69426E-13 O3S1 1.73550E-20 O3 1.00000E-30
C1H1O2 9.05180E-13 C4H6_1 1.14077E-20 S7 1.00000E-30
S 7.19264E-13 O 6.56732E-21 S8 1.00000E-30
S3 1.46179E-13 C4H6_3 6.48690E-21
POLY_3:Hit RETURN to continue
POLY_3: s-a-v 1 t 500 2000 50
... the command in full is SET_AXIS_VARIABLE
POLY_3: save tcex29 y
... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 1000.000
...OK

Phase Region from 1000.000 for:
GAS
Global test at 1.08000E+03 .... OK
Global test at 1.18000E+03 .... OK
Global test at 1.28000E+03 .... OK
Global test at 1.38000E+03 .... OK
Global test at 1.48000E+03 .... OK
Global test at 1.58000E+03 .... OK
Global test at 1.68000E+03 .... OK
Global test at 1.78000E+03 .... OK
Global test at 1.88000E+03 .... OK
Global test at 1.98000E+03 .... OK
Terminating at 2000.00
Calculated 103 equilibria

Phase Region from 1000.000 for:
GAS
Global test at 9.20000E+02 .... OK
Global check of adding phase at 8.35809E+02
Calculated 19 equilibria

Phase Region from 835.809 for:
GAS
GRAPHITE
Global test at 7.60000E+02 .... OK
Global test at 6.60000E+02 .... OK
Global test at 5.60000E+02 .... OK
Terminating at 500.000
Calculated 37 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex29\tcex
29.POLY3
POLY_3: post

```

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

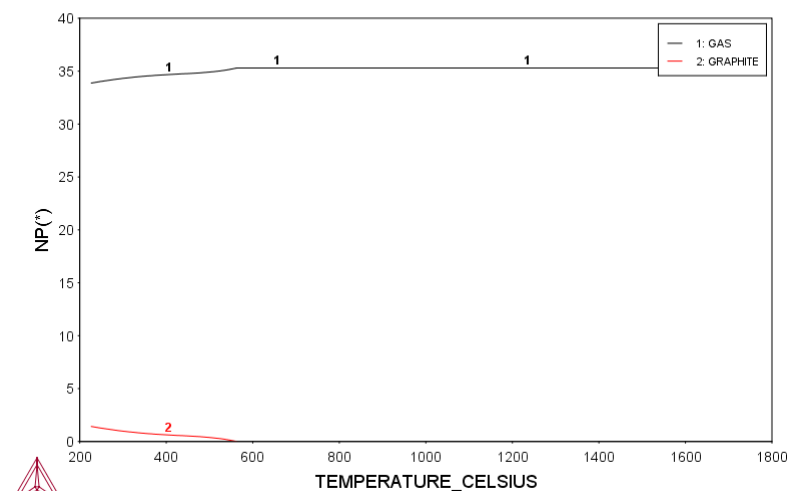
```

POST:
POST: @@ plot amount of phases, mainly gas!
POST: s-d-a x t-c
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y np(*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: s-l f
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 29a
POST: plot
... the command in full is PLOT DIAGRAM

```

**example 29a**

2016.05.16.14.03.53  
SSUB5: C, H, O, S  
N(H)=20, N(C)=5, N(O)=10.2, N(S)=0.1, P=1E5



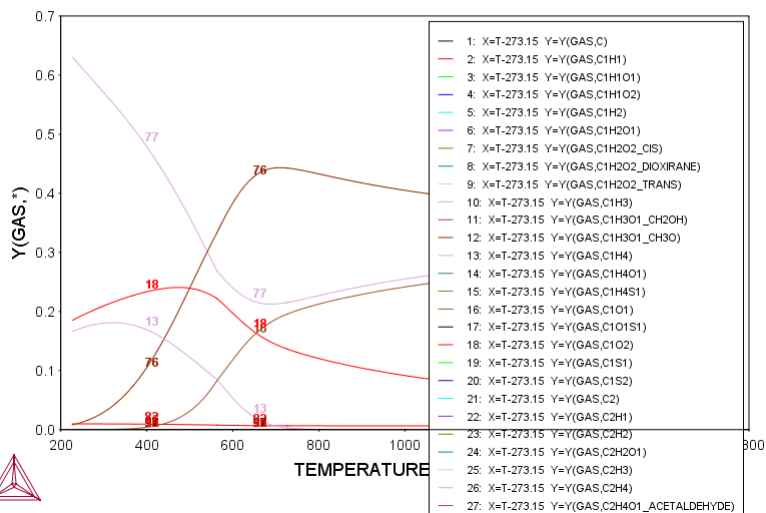
```

POST:
POST:Hit RETURN to continue
POST: @@ plot gas speciation. y(gas,*) are partial
POST: @@ pressures expressed in bar (as total pressure
POST: @@ is one bar!). Set labels on the lines.
POST: s-d-a y y(gas,*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/:
POST: set-title example 29b
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

# example 29b

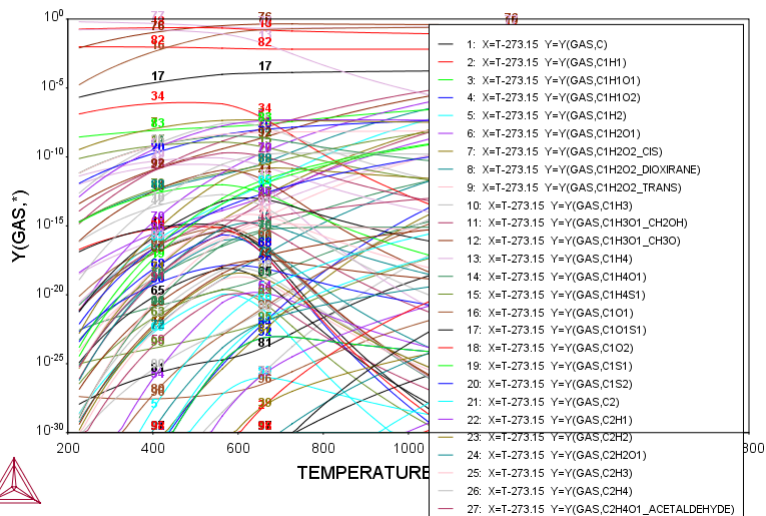
2016.05.16.14.03.54  
SSUB5: C, H, O, S  
N(H)=20., N(C)=5., N(O)=10.2, N(S)=0.1, P=1E5



```
POST:
POST:Hit RETURN to continue
POST: @@ Set logarithmic axis
POST: s-ax-ty
... the command in full is SET_AXIS_TYPE
AXIS (X, Y OR Z) : y
AXIS TYPE /LINEAR/: log
POST:
POST: set-title example 29c
POST:
POST: plot
... the command in full is PLOT DIAGRAM
```

# example 29c

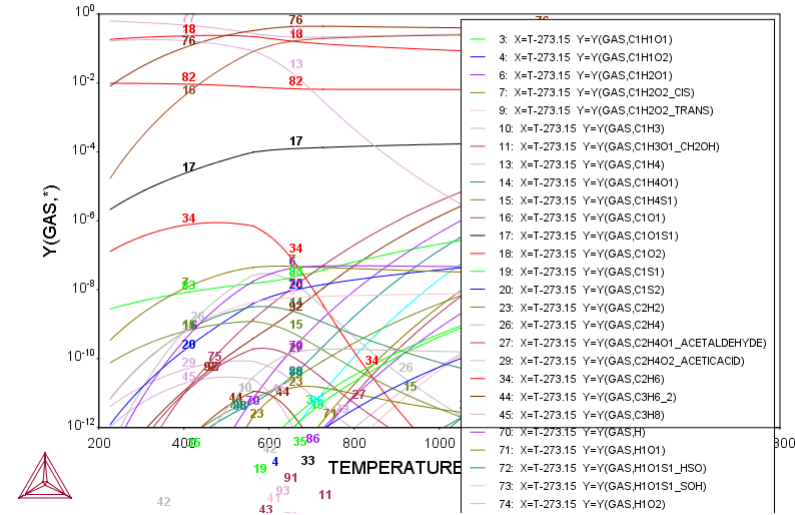
2016.05.16.14.03.59  
SSUB5: C, H, O, S  
N(H)=20., N(C)=5., N(O)=10.2, N(S)=0.1, P=1E5



```
POST:
POST:Hit RETURN to continue
POST: @@ Set scaling
POST: s-s y n 1e-12 l
... the command in full is SET_SCALING_STATUS
POST: set-title example 29d
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
```

example 29d

2016.05.16 14.04.01  
SSUBS: C, H, O, S  
N(H)=20., N(C)=5., N(O)=10.2, N(S)=0.1, P=1E5



POST:  
POST: set-inter  
... the command in full is SET\_INTERACTIVE\_MODE  
POST:

tcex30A

About Stockholm, Sweden

Software (build 9533) running on WinNT 64-bit wordlength  
Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118  
License library version: 8.5.1.0017  
Linked: Mon May 16 09:31:44 2016

SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex30A\tcex30A.TCM"SYS: set-echo

SYS: @@  
SYS: @@  
SYS: @@ Example of Scheil calculation for Al-4Mg-2Si-2Cu  
SYS: @@ Part A: step-by-step calculation  
SYS: @@

SYS:  
SYS: go da  
THERMODYNAMIC DATABASE module  
Current database: Steels/Fe-Alloys v8.0

VA DEFINED  
L12\_FCC B2\_BCC B2\_VACANCY  
HIGH\_SIGMA DICTRA\_FCC\_A1 REJECTED

TDB\_TCFE8: sw user tcex30\_cost2.TDB  
Current database: User defined Database  
This database does not support the DATABASE\_INFORMATION command

VA /- DEFINED  
TDB\_USER: def-ele al cu mg si MG  
AL CU  
SI DEFINED  
TDB\_USER: get  
ELEMENTS .....  
SPECIES .....  
PHASES .....  
PARAMETERS ...  
Reference REF1 missing close to line 765  
Reference REF1 missing close to line 767  
Reference REF1 missing close to line 769  
Reference REF1 missing close to line 771  
FUNCTIONS ....

List of references for assessed data

'COST2 - TCOST507 Light Alloys Database (Version 2.1), provided by TCSAB,  
1999/2003. '  
-OK-

TDB\_USER: go p-3

POLY version 3.32  
POLY\_3: s-c p=101325 n=1 t=1000 w(si)=0.02 w(mg)=0.04 w(cu)=0.02  
POLY\_3: c-e

Using global minimization procedure  
Calculated 24550 grid points in 0 s  
Found the set of lowest grid points in 0 s  
Calculated POLY solution 0 s, total time 0 s

POLY\_3: l-e,,  
Options /VWCS/:  
Output from POLY-3, equilibrium = 1, label A0 , database: USER

Conditions:  
P=1.01325E5, N=1, T=1000, W(SI)=2E-2, W(MG)=4E-2, W(CU)=2E-2  
DEGREES OF FREEDOM 0

Temperature 1000.00 K ( 726.85 C), Pressure 1.013250E+05  
Number of moles of components 1.00000E+00, Mass in grams 2.71965E+01  
Total Gibbs energy -4.56562E+04, Enthalpy 3.06144E+04, Volume 0.00000E+00

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
AL	9.2731E-01	9.2000E-01	5.4982E-03	-4.3263E+04	SER
CU	8.5596E-03	2.0000E-02	5.9020E-07	-1.1925E+05	SER
MG	4.4759E-02	4.0000E-02	1.0064E-04	-7.6526E+04	SER
SI	1.9367E-02	2.0000E-02	1.1370E-03	-5.6367E+04	SER

LIQUID Status ENTERED Driving force 0.0000E+00  
Moles 1.0000E+00, Mass 2.7197E+01, Volume fraction 0.0000E+00 Mass fractions:  
AL 9.20000E-01 MG 4.00000E-02 CU 2.00000E-02 SI 2.00000E-02

POLY\_3: @@ calculate liquidus temperature in order to choose  
POLY\_3: @@ a starting temperature where only liquid exists  
POLY\_3: c-st phase fcc\_al=fix 0

POLY\_3: s-c t=none  
POLY\_3: c-e  
Normal POLY minimization, not global  
Testing POLY result by global minimization procedure  
Calculated 24550 grid points in 0 s  
12 ITS, CPU TIME USED 0 SECONDS

POLY\_3: l-e,,  
Options /VWCS/:  
Output from POLY-3, equilibrium = 1, label A0 , database: USER

Conditions:  
P=1.01325E5, N=1, W(SI)=2E-2, W(MG)=4E-2, W(CU)=2E-2  
FIXED PHASES  
FCC\_A1=0  
DEGREES OF FREEDOM 0

Temperature 897.74 K ( 624.59 C), Pressure 1.013250E+05  
Number of moles of components 1.00000E+00, Mass in grams 2.71965E+01  
Total Gibbs energy -3.80281E+04, Enthalpy 2.73862E+04, Volume 0.00000E+00

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
AL	9.2731E-01	9.2000E-01	8.2190E-03	-3.5838E+04	SER
CU	8.5596E-03	2.0000E-02	5.5836E-07	-1.0747E+05	SER
MG	4.4759E-02	4.0000E-02	1.2754E-04	-6.6933E+04	SER
SI	1.9367E-02	2.0000E-02	2.2867E-03	-4.5388E+04	SER

LIQUID Status ENTERED Driving force 0.0000E+00  
Moles 1.0000E+00, Mass 2.7197E+01, Volume fraction 0.0000E+00 Mass fractions:  
AL 9.20000E-01 MG 4.00000E-02 CU 2.00000E-02 SI 2.00000E-02

FCC\_A1 Status FIXED Driving force 0.0000E+00  
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mass fractions:

```

AL 9.85194E-01 MG 1.12509E-02 CU 1.91685E-03 SI 1.63879E-03
POLY_3: show t
T=897.74074
POLY_3:Hit RETURN to continue
POLY_3: s-c t
Value /897.7407448/: 900
POLY_3: c-st phase
Phase name(s): fcc_al
Status: /ENTERED/: ENTERED
Start value, number of moles /0/: 0
POLY_3: c-e
Using global minimization procedure
Calculated 24550 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY_3: l-e,,
Options /VWCS/:
Output from POLY-3, equilibrium = 1, label A0 , database: USER

Conditions:
P=1.01325E5, N=1, T=900, W(SI)=2E-2, W(MG)=4E-2, W(CU)=2E-2
DEGREES OF FREEDOM 0

Temperature 900.00 K ( 626.85 C), Pressure 1.013250E+05
Number of moles of components 1.00000E+00, Mass in grams 2.71965E+01
Total Gibbs energy -3.81928E+04, Enthalpy 2.74567E+04, Volume 0.00000E+00

Component      Moles      W-Fraction Activity Potential Ref.stat
AL              9.2731E-01  9.2000E-01  8.1424E-03 -3.5998E+04 SER
CU              8.5596E-03  2.0000E-02  5.5930E-07 -1.0773E+05 SER
MG              4.4759E-02  4.0000E-02  1.2687E-04 -6.7141E+04 SER
SI              1.9367E-02  2.0000E-02  2.2488E-03 -4.5627E+04 SER

LIQUID          Status ENTERED Driving force 0.0000E+00
Moles 1.0000E+00, Mass 2.7197E+01, Volume fraction 0.0000E+00 Mass fractions:
AL 9.20000E-01 MG 4.00000E-02 SI 2.00000E-02 CU 2.00000E-02
POLY_3: s-a-v 1 t
Min value /0/: 750 900 1
POLY_3:
POLY_3: ent var nl=1;
POLY_3: ent var nfcc=0;
POLY_3: ent var nl=np(liquid)*nl;
POLY_3: ent fun ns=1-nl;
POLY_3: ent var nfcc=nfcc+nl*np(fcc_al);
POLY_3: ent var wsi=w(liquid,si);
POLY_3: ent var wmg=w(liquid,mg);
POLY_3: ent var wcu=w(liquid,cu);
POLY_3: ent tab tabl
Variable(s): t nl ns nfcc
&
POLY_3: s-c w(si)=wsi w(mg)=wmg w(cu)=wcu
POLY_3: save tcex30a y
POLY_3:
POLY_3: step
Option? /NORMAL/: eva
Variable name(s): wsi wmg wcu
No initial equilibrium, using default
...OK

Phase Region from 900.000 for:
LIQUID
Global check of adding phase at 8.97741E+02
Calculated 5 equilibria

Phase Region from 897.741 for:
LIQUID
FCC_A1
Global test at 8.90000E+02 .... OK
Global test at 8.80000E+02 .... OK
Global test at 8.70000E+02 .... OK
Global test at 8.60000E+02 .... OK
Global check of adding phase at 8.57875E+02
Calculated 43 equilibria

Phase Region from 857.875 for:
LIQUID
FCC_A1
MG2SI
Global test at 8.50000E+02 .... OK
Global test at 8.40000E+02 .... OK
Global test at 8.30000E+02 .... OK
Global test at 8.20000E+02 .... OK
Global test at 8.10000E+02 .... OK
Global test at 8.00000E+02 .... OK
Global test at 7.90000E+02 .... OK
Global test at 7.80000E+02 .... OK
Global check of adding phase at 7.78888E+02
Calculated 82 equilibria

Phase Region from 778.888 for:
LIQUID
ALCU_THETA
FCC_A1
MG2SI
Global check of adding phase at 7.73208E+02
Calculated 8 equilibria

Phase Region from 773.208 for:
LIQUID
ALCU_THETA
DIAMOND_A4
FCC_A1
MG2SI
Calculated 2 equilibria

Phase Region from 773.208 for:
ALCU_THETA
DIAMOND_A4
FCC_A1
MG2SI
Global test at 7.66000E+02 .... OK
Global test at 7.56000E+02 .... OK
Terminating at 750.000
Calculated 27 equilibria

```

```
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex30A\tce
x30a.POLY3
POLY_3:
POLY_3: post
```

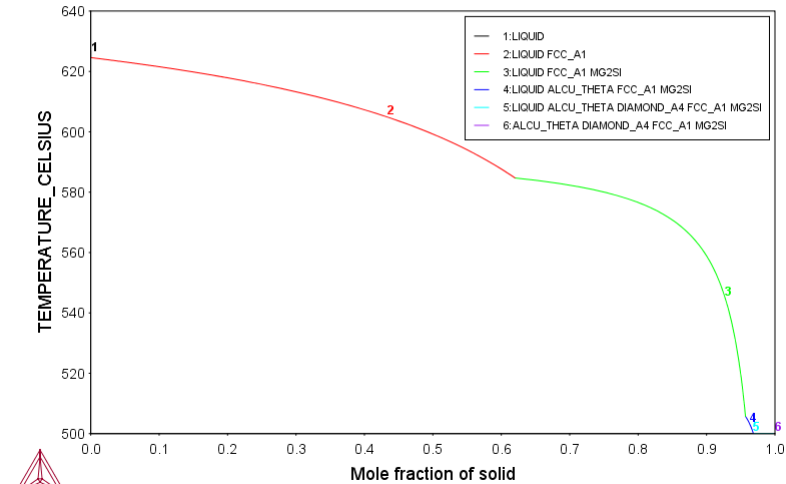
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

```
POST: s-d-a x tab1
COLUMN NUMBER /*/: 3
POST: s-d-a y t-c
POST:
POST: s-s-s y
AUTOMATIC SCALING (Y OR N) /N/: n
MIN VALUE : 500 640
POST: s-lab b
POST: se-ax-te x n
AXIS TEXT : Mole fraction of solid
POST: set-title example 30Aa
POST: plot
```

example 30Aa

2016.05.16.14.05.39  
USER: AL, CU, MG, SI  
P=1.01325E5, N=1., W(SI)=WSI, W(MG)=WMG, W(CU)=WCU



```
POST:
POST: Hit RETURN to continue
POST: back
POLY_3: read,,
POLY_3: po
```

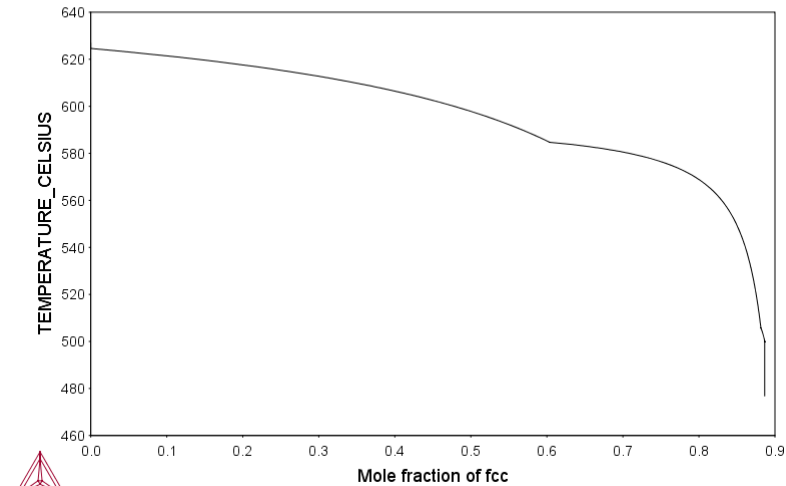
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

```
POST: s-d-a x tab1
COLUMN NUMBER /*/: 4
POST: s-d-a y t-c
POST: se-ax-te x n
AXIS TEXT : Mole fraction of fcc
POST: set-title example 30Ab
POST:
POST: plot
```

example 30Ab

2016.05.16.14.05.40  
USER: AL, CU, MG, SI  
P=1.01325E5, N=1, W(SI)=WSI, W(MG)=WMG, W(CU)=WCU

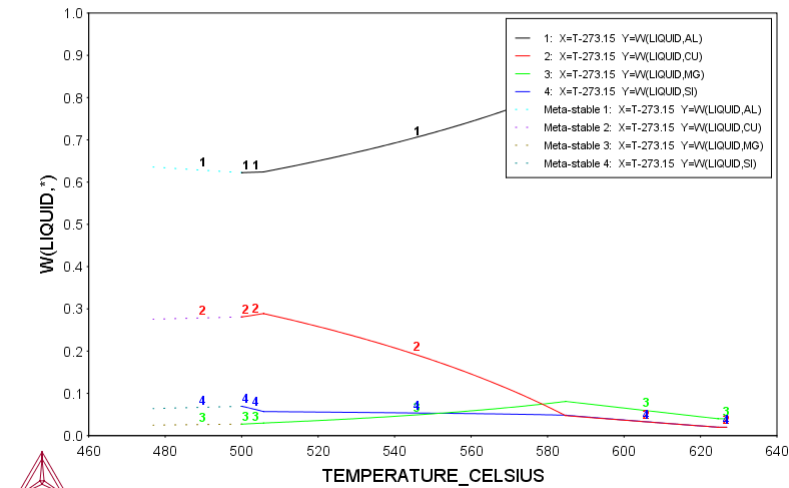


```
POST:
POST: Hit RETURN to continue
POST: s-d-a x t-c
POST: s-d-a y w(liquid,*),,
POST: set-title example 30Ac
```

POST: s-l d  
POST:  
POST: plot

example 30Ac

2016.05.16.14.05.41  
USER: AL, CU, MG, SI  
P=1.01325E5, N=1, W(SI)=WSI, W(MG)=WMG, W(CU)=WCU



POST:  
POST: set-inter  
POST:



tcex30B

About Linked: Mon May 16 09:31:44 2016

```
SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex30B\tcex30B.TCM"SYS: set-echo
SYS: @@
SYS: @@
SYS: @@ Example of Scheil calculation for Al-4Mg-2Si-2Cu
SYS: @@ Part B: using SCHEIL module
SYS: @@
SYS: set-log ex30,,,
SYS:
SYS: go scheil
... the command in full is GOTO_MODULE
SCHEIL: start
... the command in full is START_WIZARD
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
L12_FCC B2_BCC B2_VACANCY
HIGH_SIGMA DICTRA_FCC_A1 REJECTED
Database /TCFE8/: user tcex30_cost2.TDB
Current database: User defined Database
This database does not support the DATABASE_INFORMATION command

VA /- DEFINED
Major element or alloy: al
Composition input in mass (weight) percent? /Y/:
1st alloying element: mg 4 si 2 cu 2
Next alloying element:
Temperature (C) /2000/: 800
VA /- DEFINED
REINITIATING GES5 .....
... the command in full is DEFINE_ELEMENTS
AL DEFINED
... the command in full is DEFINE_ELEMENTS
MG DEFINED
... the command in full is DEFINE_ELEMENTS
SI DEFINED
... the command in full is DEFINE_ELEMENTS
CU DEFINED

This database has following phases for the defined system

LIQUID:L AL12MG17 ALCE_AMORPHOUS
ALCUZN_T ALCU_DELTA ALCU_EPSILON
ALCU_ETA ALCU_PRIME ALCU_THETA
ALCU_ZETA ALLI ALMG_BETA
ALMG_EPS ALMG_GAMMA ALMO
ALM_D019 ALND_AMORPHOUS ALTI
BCC_A2 BCC_B2 BCT_A5
CBCC_A12 CR3SI_A15 CRSI2
CU19SI6_ETA CU33SI7_DELTA CU4SI_EPSILON
CU56SI11_GAMMA CU6Y CUB_A13
CUB_A15 CUMG2 CUMGSI_SIGMA
CUMGSI_TAU CUZN_GAMMA DIAMOND_A4
FCC_A1 GAMMA_D83 GAMMA_H
HCP_A3 HCP_ZN LAVES_C14
LAVES_C15 LAVES_C36 MG24Y5
MG2SI MG2Y MG2ZN11
MG2ZN3 MGY_GAMMA MGZN
PHI QPHASE SIV3
SPHASE TAU VPHASE

Reject phase(s) /NONE/: *
LIQUID:L AL12MG17 ALCE_AMORPHOUS
ALCUZN_T ALCU_DELTA ALCU_EPSILON
ALCU_ETA ALCU_PRIME ALCU_THETA
ALCU_ZETA ALLI ALMG_BETA
ALMG_EPS ALMG_GAMMA ALMO
ALM_D019 ALND_AMORPHOUS ALTI
BCC_A2 BCC_B2 BCT_A5
CBCC_A12 CR3SI_A15 CRSI2
CU19SI6_ETA CU33SI7_DELTA CU4SI_EPSILON
CU56SI11_GAMMA CU6Y CUB_A13
CUB_A15 CUMG2 CUMGSI_SIGMA
CUMGSI_TAU CUZN_GAMMA DIAMOND_A4
FCC_A1 GAMMA_D83 GAMMA_H
HCP_A3 HCP_ZN LAVES_C14
LAVES_C15 LAVES_C36 MG24Y5
MG2SI MG2Y MG2ZN11
MG2ZN3 MGY_GAMMA MGZN
PHI QPHASE SIV3
SPHASE TAU VPHASE
REJECTED
Restore phase(s):: liquid fcc_al alcu_th mg2si diamond_a4 all2mg17
LIQUID:L FCC_A1 ALCU_THETA
MG2SI DIAMOND_A4 AL12MG17
RESTORED
Restore phase(s): /NONE/:

.....

The following phases are retained in this system:

LIQUID:L AL12MG17 ALCU_THETA
DIAMOND_A4 FCC_A1 MG2SI

.....

OK? /Y/: Y
*** GAS INPUT IGNORED
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
Reference REF1 missing close to line 765
Reference REF1 missing close to line 767
Reference REF1 missing close to line 769
```

Reference REF1 missing close to line 771  
FUNCTIONS ....

List of references for assessed data

'COST2 - TCOST507 Light Alloys Database (Version 2.1), provided by TCSAB,  
1999/2003. '

-OK-

Should any phase have a miscibility gap check? /N/: N

LIQUID PHASE NAME: LIQUID

Fast diffusing components: /NONE/:

... the command in full is SET\_NUMERICAL\_LIMITS

... the command in full is COMPUTE\_TRANSITION

This command is a combination of CHANGE\_STATUS and SET\_CONDITION

to calculate directly when a phase may form by releasing one condition.

You must release one of these conditions

T=1073.15, W(MG)=4E-2, W(SI)=2E-2, W(CU)=2E-2, P=1E5, N=1

DEGREES OF FREEDOM 0

To form FCC\_A1#1 the condition is set to T=897.740744839

CALCULATING USING NORMAL EQUILIBRIUM CONDITIONS

... the command in full is ADD\_INITIAL\_EQUILIBRIUM

... the command in full is ADVANCED\_OPTIONS

... the command in full is STEP\_WITH\_OPTIONS

...OK

Phase Region from 897.731 for:

LIQUID

FCC\_A1

Global Check of removing phase at 8.97741E+02

Calculated 3 equilibria

Phase Region from 897.741 for:

LIQUID

Terminating at 897.831

Calculated 4 equilibria

Phase Region from 897.731 for:

LIQUID

FCC\_A1

Global test at 8.89731E+02 .... OK

Global test at 8.79731E+02 .... OK

Global test at 8.69731E+02 .... OK

Global test at 8.59731E+02 .... OK

Global check of adding phase at 8.57535E+02

Calculated 43 equilibria

Phase Region from 857.535 for:

LIQUID

FCC\_A1

MG2SI

Global test at 8.49731E+02 .... OK

Global test at 8.39731E+02 .... OK

Global test at 8.29731E+02 .... OK

Global check of removing phase at 8.26196E+02

Calculated 34 equilibria

Phase Region from 826.196 for:

FCC\_A1

MG2SI

Calculated 4 equilibria

\*\*\* Buffer saved on file:

c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex30B\SCH

EIL\_676.POLY3

POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

... the command in full is ENTER\_SYMBOL

... the command in full is MAKE\_EXPERIMENTAL\_DATAFI

An EXP file c:\jenkins\workspace\1\THERMO\1\examples\tcex30B\SCHEIL\_EQ\_676.EXP

has been created to store the equilibrium solidification results.

... the command in full is READ\_WORKSPACES

CALCULATING SCHEIL SOLIDIFICATION

... the command in full is SET\_NUMERICAL\_LIMITS

T(C) fraction solid

624.6807 0.000000

PHASE REGION:LIQUID + FCC\_A1

T(C) fraction solid

624.5870 0.1358787E-03

623.5870 0.3532418E-01

622.5870 0.6836458E-01

621.5870 0.9944066E-01

620.5870 0.1287161

619.5870 0.1563371

618.5870 0.1824349

617.5870 0.2071274

616.5870 0.2305208

615.5870 0.2527111

614.5870 0.2737852

613.5870 0.2938222

612.5870 0.3128937

611.5870 0.3310652

610.5870 0.3483963

609.5870 0.3649419

608.5870 0.3807520

607.5870 0.3958726

606.5870 0.4103460

605.5870 0.4242113

604.5870 0.4375043

603.5870 0.4502583

602.5870 0.4625042

601.5870 0.4742703

600.5870 0.4855831

599.5870	0.4964672
598.5870	0.5069455
597.5870	0.5170392
596.5870	0.5267681
595.5870	0.5361509
594.5870	0.5452047
593.5870	0.5539459
592.5870	0.5623895
591.5870	0.5705498
590.5870	0.5784402
589.5870	0.5860731
588.5870	0.5934603
587.5870	0.6006129
586.5870	0.6075414
585.5870	0.6142556
584.7432	0.6197601

PHASE REGION:LIQUID + FCC\_A1 + MG2SI

T(C)	fraction solid
584.7120	0.6204291
583.7120	0.6580982
582.7120	0.6889903
581.7120	0.7147690
580.7120	0.7365965
579.7120	0.7553093
578.7120	0.7715239
577.7120	0.7857051
576.7120	0.7982095
575.7120	0.8093153
574.7120	0.8192426
573.7120	0.8281678
572.7120	0.8362341
571.7120	0.8435586
570.7120	0.8502382
569.7120	0.8563537
568.7120	0.8619730
567.7120	0.8671536
566.7120	0.8719445
565.7120	0.8763876
564.7120	0.8805191
563.7120	0.8843705
562.7120	0.8879691
561.7120	0.8913386
560.7120	0.8945002
559.7120	0.8974722
558.7120	0.9002713
557.7120	0.9029118
556.7120	0.9054068
555.7120	0.9077679
554.7120	0.9100055
553.7120	0.9121290
552.7120	0.9141468
551.7120	0.9160667
550.7120	0.9178954
549.7120	0.9196393
548.7120	0.9213042
547.7120	0.9228952
546.7120	0.9244172
545.7120	0.9258745
544.7120	0.9272712
543.7120	0.9286109
542.7120	0.9298971
541.7120	0.9311328
540.7120	0.9323211
539.7120	0.9334645
538.7120	0.9345656
537.7120	0.9356266
536.7120	0.9366498
535.7120	0.9376371
534.7120	0.9385904
533.7120	0.9395114
532.7120	0.9404018
531.7120	0.9412630
530.7120	0.9420964
529.7120	0.9429035
528.7120	0.9436854
527.7120	0.9444432
526.7120	0.9451783
525.7120	0.9458914
524.7120	0.9465837
523.7120	0.9472560
522.7120	0.9479092
521.7120	0.9485441
520.7120	0.9491615
519.7120	0.9497621
518.7120	0.9503466
517.7120	0.9509157
516.7120	0.9514700
515.7120	0.9520100
514.7120	0.9525364
513.7120	0.9530496
512.7120	0.9535502
511.7120	0.9540386
510.7120	0.9545153
509.7120	0.9549808
508.7120	0.9554354
507.7120	0.9558795
506.7120	0.9563136
505.7432	0.9567248

PHASE REGION:LIQUID + ALCU\_THETA + FCC\_A1 + MG2SI

T(C)	fraction solid
505.7120	0.9568034
504.7120	0.9595410
503.7120	0.9618872
502.7120	0.9639256
501.7120	0.9657170
500.7120	0.9673065

PHASE REGION:ALCU\_THETA + DIAMOND\_A4 + FCC\_A1 + MG2SI

T(C)	fraction solid
------	----------------

500.0557 1.0000000

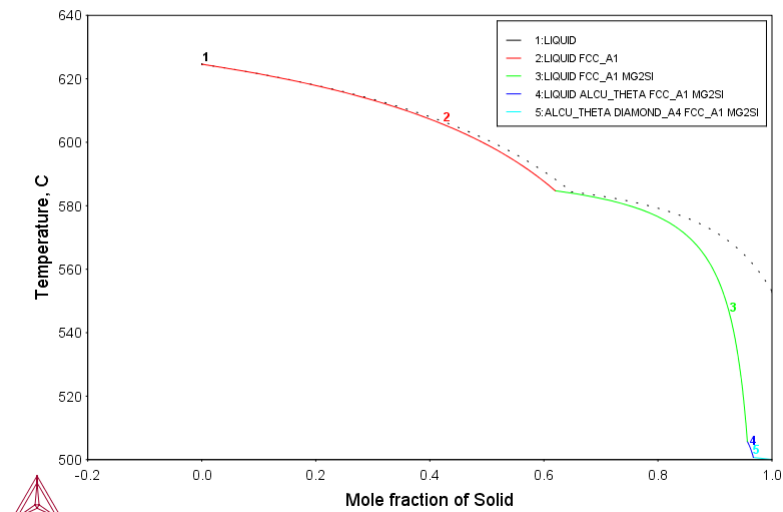
Hint: move the last function to the first equilibrium where it is used

... the command in full is SET\_LABEL\_CURVE\_OPTION  
... the command in full is APPEND EXPERIMENTAL DATA

2016.05.16.14.07.47

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 command in full is APPEND\_EXPERIMENTAL\_DATA

.....

The following axis variables are available

T --- Temperature in Celsius  
NL/BL --- Mole/mass fraction of liquid  
NS/BS --- Mole/mass fraction of all solid phases  
NS(ph)/BS(ph) --- Mole/mass fraction of a solid phase  
W(ph,el) --- Weight fraction of an element in a phase  
X(ph,el) --- Mole fraction of an element in a phase  
Y(ph,el) --- Site fraction of an element in a phase  
NN(ph,el) --- Distribution of an element in a phases  
NH/BH --- Heat release and Latent heat per mole/gram  
CP/BCP --- Apparent heat capacity per mole/gram  
NV/NV(ph) --- Molar volume of the system or a phase  
DS/DS(ph) --- Average density of the system or a phase  
BT --- Apparent volumetric TEC of the system

"el" and "ph" are name of element and phase, respectively  
"\*" can be used as a wild character for "el" and "ph"

.....

POST:

POST:Hit RETURN to continue

POST: s-d-a x t

... the command in full is SET\_DIAGRAM\_AXIS

POST: s-d-a y w(liquid,\*),,,,,,

... the command in full is SET\_DIAGRAM\_AXIS

POST: s-s-s y n 0 0.3

... the command in full is SET\_SCALING\_STATUS

POST: set-lab F

... the command in full is SET\_LABEL\_CURVE\_OPTION

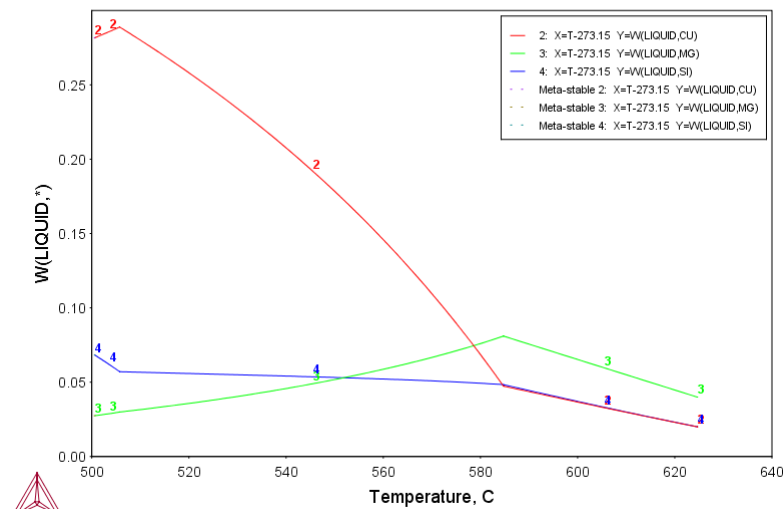
POST: plot,,,,,

... the command in full is PLOT DIAGRAM

2016.05.16.14.07.48

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

... the command in full is SET\_INTERACTIVE\_MODE

POST:



tcex31

AboutMACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex31\tcex31.TCM" set-echo

```
SYS: @@
SYS: @@
SYS: @@ Calculations of CVM and comparisons with sublattices
SYS: @@ of a fictitious A B system.
SYS: @@ Also shows how to overlay diagrams from two calculations
SYS: @@
SYS:
SYS: set-log ex31,,,
SYS:
SYS: go g
... the command in full is GOTO_MODULE
GIBBS ENERGY SYSTEM version 5.2
GES:
GES: @@ Enter the elements and their reference states
GES: e-e A B
... the command in full is ENTER_ELEMENT
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
L12_FCC          B2_BCC          B2_VACANCY
HIGH_SIGMA      DICTRA_FCC_A1   REJECTED
GES: a-e-d A
... the command in full is AMEND_ELEMENT_DATA
NEW STABLE ELEMENT REFERENCE /UNKNOWN/: FCC
NEW ATOMIC MASS /0/: 10
NEW H(298.15)-H(0) /0/: 0
NEW S(298.15) /0/: 0
Default element reference state symbol index /1/: 1
GES: a-e-d B
... the command in full is AMEND_ELEMENT_DATA
NEW STABLE ELEMENT REFERENCE /BETA_RHOMBO_B/: FCC
NEW ATOMIC MASS /10.811/: 10
NEW H(298.15)-H(0) /1222/: 0
NEW S(298.15) /5.9/: 0
Default element reference state symbol index /1/: 1
GES:
GES: @@ =====
GES: @@ These species represent the clusters. 4 clusters A3B are needed
GES: @@ as the B atom can be on 4 different sublattices etc.
GES: e-sp S0 A
... the command in full is ENTER_SPECIES
GES: e-sp S11 A.75B.25
... the command in full is ENTER_SPECIES
GES: e-sp S12 A.75B.25
... the command in full is ENTER_SPECIES
GES: e-sp S13 A.75B.25
... the command in full is ENTER_SPECIES
GES: e-sp S14 A.75B.25
... the command in full is ENTER_SPECIES
GES: e-sp S21 A.5B.5
... the command in full is ENTER_SPECIES
GES: e-sp S22 A.5B.5
... the command in full is ENTER_SPECIES
GES: e-sp S23 A.5B.5
... the command in full is ENTER_SPECIES
GES: e-sp S24 A.5B.5
... the command in full is ENTER_SPECIES
GES: e-sp S25 A.5B.5
... the command in full is ENTER_SPECIES
GES: e-sp S26 A.5B.5
... the command in full is ENTER_SPECIES
GES: e-sp S31 A.25B.75
... the command in full is ENTER_SPECIES
GES: e-sp S32 A.25B.75
... the command in full is ENTER_SPECIES
GES: e-sp S33 A.25B.75
... the command in full is ENTER_SPECIES
GES: e-sp S34 A.25B.75
... the command in full is ENTER_SPECIES
GES: e-sp S4 B
... the command in full is ENTER_SPECIES
GES:
GES: @@ =====
GES: @@ This function describes the bond energy A-B at equiatomic composition
GES: e-sy fun UIJ
... the command in full is ENTER_SYMBOL
LOW TEMPERATURE LIMIT /298.15/: 298.15
FUNCTION: -100*R;
HIGH TEMPERATURE LIMIT /6000/: 6000
ANY MORE RANGES /N/: N
GES:
GES: @@ These functions describe the end-member energies at A3B, A2B2 and AB3
GES: @@ respectively. In the simplest case, like here, they are just the
GES: @@ bond energy multiplied with 3, 4 and 3 respectively.
GES: e-sy fun GA3B1,,3*UIJ;,,,
... the command in full is ENTER_SYMBOL
GES: e-sy fun GA2B2,,4*UIJ;,,,
... the command in full is ENTER_SYMBOL
GES: e-sy fun GA1B3,,3*UIJ;,,,
... the command in full is ENTER_SYMBOL
GES:
GES: @@ =====
GES: @@ This is the fcc phase with CVM for both lro and sro
GES: e-ph CVM_TET
... the command in full is ENTER_PHASE
TYPE CODE:
NUMBER OF SUBLATTICES /1/: 1
NAME OF CONSTITUENT: S0 S11 S12 S13 S14 S21 S22 S23 S24 S25 S26 S31 S32 S33 S34 S4
NAME OF CONSTITUENT:
WILL YOU ADD CONSTITUENTS LATER /NO/: NO
DO YOU WANT A LIST OF POSSIBLE PARAMETERS /NO/: NO
GES: E-PAR G(C,S11),,GA3B1;,,,
... the command in full is ENTER_PARAMETER
G(CVM_TET,S11;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
GES: E-PAR G(C,S12),,GA3B1;,,,
... the command in full is ENTER_PARAMETER
G(CVM_TET,S12;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0)
```

```

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

```

10UTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT                      DATE 2016- 5-16  
FROM DATABASE: User data 2016.05.16

ALL DATA IN SI UNITS  
FUNCTIONS VALID FOR    298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

ELEMENT	STABLE	ELEMENT	REFERENCE	MASS	H298-H0	S298
1	A	FCC		1.0000E+01	0.0000E+00	0.0000E+00
2	B	FCC		1.0000E+01	0.0000E+00	0.0000E+00

SPECIES	STOICHIOMETRY
1 A	A
2 B	B
3 S0	A
4 S11	A0.75B0.25
5 S12	A0.75B0.25
6 S13	A0.75B0.25
7 S14	A0.75B0.25
8 S21	A0.5B0.5
9 S22	A0.5B0.5
10 S23	A0.5B0.5
11 S24	A0.5B0.5
12 S25	A0.5B0.5
13 S26	A0.5B0.5
14 S31	A0.25B0.75
15 S32	A0.25B0.75
16 S33	A0.25B0.75
17 S34	A0.25B0.75
18 S4	B

CVM\_TET  
CONSTITUENTS: S0,S11,S12,S13,S14,S21,S22,S23,S24,S25,S26,S31,S32,S33,S34,  
S4

```

G(CVM_TET,S0;0)-G(FCC,A;0) = 0.0
G(CVM_TET,S11;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(CVM_TET,S12;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(CVM_TET,S13;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(CVM_TET,S14;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(CVM_TET,S21;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S22;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S23;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S24;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S25;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S26;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(CVM_TET,S31;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(CVM_TET,S32;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(CVM_TET,S33;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(CVM_TET,S34;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(CVM_TET,S4;0)-G(FCC,B;0) = 0.0

```

SYMBOL	STATUS	VALUE/FUNCTION
1 R	80000000	8.3145100E+00
2 RTLNP	20000000	+R*T*LN(1E-05*P)
103 UIJ	20000000	-100*R
104 GA3B1	20000000	+3*UIJ
105 GA2B2	20000000	+4*UIJ
106 GA1B3	20000000	+3*UIJ

```

GES:
GES:Hit RETURN to continue
GES: @@ =====
GES: @@ This is an fcc phase with no sro but lro
GES: @@ described with the sublattice model
GES: E-PH LRO
... the command in full is ENTER_PHASE
TYPE CODE:
NUMBER OF SUBLATTICES /1/: 4
NUMBER OF SITES IN SUBLATTICE 1 /1/: .25
NUMBER OF SITES IN SUBLATTICE 2 /1/: .25
NUMBER OF SITES IN SUBLATTICE 3 /1/: .25

```

```

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,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,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,B:B:A:A),,GA2B2,,,,
... the command in full is ENTER_PARAMETER
G(LRO,B:B:A:A;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0)
GES: l-p-d lro
... the command in full is LIST_PHASE_DATA

LRO
EXCESS MODEL IS REDLICH-KISTER MUGGIANU
4 SUBLATTICES, SITES .25: .25: .25: .25
CONSTITUENTS: A,B : A,B : A,B : A,B

G(LRO,A:A:A:A;0)-G(FCC,A;0) = 0.0
G(LRO,B:A:A:A;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(LRO,A:B:A:A;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(LRO,B:B:A:A;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(LRO,A:A:B:A;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(LRO,B:A:B:A;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(LRO,A:B:B:A;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(LRO,B:B:B:A;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(LRO,A:A:A:B;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
G(LRO,B:A:A:B;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(LRO,A:B:A:B;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(LRO,B:B:A:B;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(LRO,A:A:B:B;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
G(LRO,B:A:B:B;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(LRO,A:B:B:B;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
G(LRO,B:B:B:B;0)-G(FCC,B;0) = 0.0

GES:
GES: @@ =====
GES: @@ This is the fcc phase with no sro and no lro. The regular
GES: @@ parameters is simply 12 times the bond energy as the ;1 and ;2
GES: @@ parameters cancel when GA1B3=GA3B1=0.75*GA2B2
GES: e-ph fcc_a1
... the command in full is ENTER_PHASE
TYPE CODE:
NUMBER OF SUBLATTICES /1/: 1
NAME OF CONSTITUENT: A B
NAME OF CONSTITUENT:
WILL YOU ADD CONSTITUENTS LATER /NO/: NO
DO YOU WANT A LIST OF POSSIBLE PARAMETERS /NO/: NO
GES:
GES: e-par l(fcc,a,b;0),,GA3B1+1.5*GA2B2+GA1B3,,,,
... the command in full is ENTER_PARAMETER
L(FCC_A1,A,B;0)
GES: e-par l(fcc,a,b;1),,2*GA3B1-2*GA1B3,,,,
... the command in full is ENTER_PARAMETER
L(FCC_A1,A,B;1)
GES: e-par l(fcc,a,b;2),,GA3B1-1.5*GA2B2+GA1B3,,,,
... the command in full is ENTER_PARAMETER
L(FCC_A1,A,B;2)
GES: l-p-d fcc
... the command in full is LIST_PHASE_DATA

FCC_A1
EXCESS MODEL IS REDLICH-KISTER MUGGIANU
CONSTITUENTS: A,B

G(FCC_A1,A;0)-G(FCC,A;0) = 0.0
G(FCC_A1,B;0)-G(FCC,B;0) = 0.0
L(FCC_A1,A,B;0) = +GA3B1+1.5*GA2B2+GA1B3
L(FCC_A1,A,B;1) = +2*GA3B1-2*GA1B3

```



```

L(FCC_A1,A,B;2) = +GA3B1-1.5*GA2B2+GA1B3
GES:
GES: @@ Finally we add together the LRO phase with the disordered FCC
GES: @@ Note that the parameters in LRO will give zero contribution
GES: @@ when the phase is disordered
GES: amend-phase LRO dis FCC
... the command in full is AMEND_PHASE_DESCRIPTION
GES:
GES: @@
GES: @@ This is the secret way to set CVM entropy calculation
GES: am-ph cvm stat 02204030
... the command in full is AMEND_PHASE_DESCRIPTION
GES:
GES: l-p-d cvm
... the command in full is LIST_PHASE_DATA

CVM_TET
$ CVM-SRO ENTROPY CONTRIBUTION
  CONSTITUENTS: S0,S11,S12,S13,S14,S21,S22,S23,S24,S25,S26,S31,S32,S33,S34,
  S4

  G(CVM_TET,S0;0)-G(FCC,A;0) = 0.0
  G(CVM_TET,S11;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
  G(CVM_TET,S12;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
  G(CVM_TET,S13;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
  G(CVM_TET,S14;0)-0.75 G(FCC,A;0)-0.25 G(FCC,B;0) = +GA3B1
  G(CVM_TET,S21;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
  G(CVM_TET,S22;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
  G(CVM_TET,S23;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
  G(CVM_TET,S24;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
  G(CVM_TET,S25;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
  G(CVM_TET,S26;0)-0.5 G(FCC,A;0)-0.5 G(FCC,B;0) = +GA2B2
  G(CVM_TET,S31;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
  G(CVM_TET,S32;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
  G(CVM_TET,S33;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
  G(CVM_TET,S34;0)-0.25 G(FCC,A;0)-0.75 G(FCC,B;0) = +GA1B3
  G(CVM_TET,S4;0)-G(FCC,B;0) = 0.0
GES:
GES:Hit RETURN to continue
GES: @@ We need 3 CVM phases for the L10, L12 and disordered states
GES: am-ph cvm
... the command in full is AMEND_PHASE_DESCRIPTION
AMEND WHAT /COMPOSITION SETS/: COMPOSITION_SETS
NEW HIGHEST SET NUMBER /2/: 3
GIVE FOR COMPOSITION SET 2
Major constituent(s) for sublattice 1: /$/: s11
GIVE FOR COMPOSITION SET 3
Major constituent(s) for sublattice 1: /$/: none
GES:
GES: am-ph cvm maj
... the command in full is AMEND_PHASE_DESCRIPTION
Composition set /1/: 1
Major constituent(s) for sublattice 1: /S0 S11 S12 S13 S14 S21 S22 S23 S24 S25 S26 S31 S32 S33 S34 S/: S25
GES:
GES: @@ Also for the sublattice phase we need 3 composition sets
GES: am-ph lro
... the command in full is AMEND_PHASE_DESCRIPTION
AMEND WHAT /COMPOSITION SETS/: COMPOSITION_SETS
NEW HIGHEST SET NUMBER /2/: 3
GIVE FOR COMPOSITION SET 2
Major constituent(s) for sublattice 1: /A B/: *
Major constituent(s) for sublattice 2: /A B/: *
Major constituent(s) for sublattice 3: /A B/: *
Major constituent(s) for sublattice 4: /A B/: *
GIVE FOR COMPOSITION SET 3
Major constituent(s) for sublattice 1: /A B/: A
Major constituent(s) for sublattice 2: /A B/: A
Major constituent(s) for sublattice 3: /A B/: B
Major constituent(s) for sublattice 4: /A B/: B
GES: am-ph lro
... the command in full is AMEND_PHASE_DESCRIPTION
AMEND WHAT /COMPOSITION SETS/: maj
Composition set /1/: 1
Major constituent(s) for sublattice 1: /A B/: A
Major constituent(s) for sublattice 2: /A B/: A
Major constituent(s) for sublattice 3: /A B/: A
Major constituent(s) for sublattice 4: /A B/: B
GES:
GES: l-d,,,
... the command in full is LIST_DATA

```

```

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT      DATE 2016- 5-16
FROM DATABASE: User data 2016.05.16

```

ALL DATA IN SI UNITS  
FUNCTIONS VALID FOR 298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

ELEMENT	STABLE	ELEMENT	REFERENCE	MASS	H298-H0	S298
1	A	FCC		1.00000E+01	0.00000E+00	0.00000E+00
2	B	FCC		1.00000E+01	0.00000E+00	0.00000E+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;0) = 0.0
  G(LRO,B:A:A;0) = +GA3B1
  G(LRO,A:B:A;0) = +GA3B1
  G(LRO,B:B:A;0) = +GA2B2
  G(LRO,A:A:B;0) = +GA3B1
  G(LRO,B:A:B;0) = +GA2B2
  G(LRO,A:B:B;0) = +GA2B2
  G(LRO,B:B:B;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) = +GA1B3
  G(LRO,B:B:B;B;0) = 0.0

```

SYMBOL	STATUS	VALUE/FUNCTION
1 R	80000000	8.3145100E+00
2 RTLNP	20000000	+R*T*LN(1E-05*P)
103 UIJ	20000000	-100*R
104 GA3B1	20000000	+3*UIJ
105 GA2B2	20000000	+4*UIJ
106 GA1B3	20000000	+3*UIJ

GES:Hit RETURN to continue

GES: @@ =====

GES: @@ Now we can start calculating

GES: go p-3

... the command in full is GOTO\_MODULE

POLY version 3.32

POLY\_3:

POLY\_3: @@ turn global minimization off

POLY\_3: set-min-op

... the command in full is SET\_MINIMIZATION\_OPTIONS

This command is DEPRECATED and to be removed in the future!

Settings for global minimization:

Use global minimization /Y/: n

Settings for general calculations:

Force positive definite Phase Hessian /Y/: n

Control minimization step size /Y/:

POLY\_3:

POLY\_3: L-C

... the command in full is LIST\_CONDITIONS

DEGREES OF FREEDOM 4

POLY\_3: S-C T=60 P=1E5 N=1 X(B)=.4

... the command in full is SET\_CONDITION

POLY\_3: @@

POLY\_3: @@ First calculate just with the full CVM phases

POLY\_3: ch-st ph \*=sus

... the command in full is CHANGE\_STATUS

POLY\_3: ch-st ph cvm cvm#2 cvm#3=ent 1

... the command in full is CHANGE\_STATUS

POLY\_3: @@

POLY\_3: @@ L10 ordering, setting start composition essential ....

POLY\_3: @@ The initial fraction of each species is bascially calculated as the

POLY\_3: @@ product of the site fraction on each sublattice.

POLY\_3: s-s-c cvm

... the command in full is SET\_START\_CONSTITUTION

Y(CVM\_TET,S0) /1/: .002

Y(CVM\_TET,S11) /1/: 1.16e-3

Y(CVM\_TET,S12) /1/: 1.76e-1

Y(CVM\_TET,S13) /1/: 1.16e-3

Y(CVM\_TET,S14) /1/: 1.76e-1

Y(CVM\_TET,S21) /1/: 7.56e-3

Y(CVM\_TET,S22) /1/: 5e-5

Y(CVM\_TET,S23) /1/: 7.56e-3

Y(CVM\_TET,S24) /1/: 7.56e-3

```

Y(CVM_TET,S25) /1/: 6.08e-1
Y(CVM_TET,S26) /1/: 7.56e-3
Y(CVM_TET,S31) /1/: 1.76e-3
Y(CVM_TET,S32) /1/: 2e-5
Y(CVM_TET,S33) /1/: 1.76e-3
Y(CVM_TET,S34) /1/: 2e-5
Y(CVM_TET,S4) /1/: 4e-7
POLY_3:
POLY_3: @@ L12 ordering
POLY_3: s-s-c cvm#2
... the command in full is SET_START_CONSTITUTION
Y(CVM_TET#2,S0) /1/: .002
Y(CVM_TET#2,S11) /1/: .46
Y(CVM_TET#2,S12) /1/: .0078
Y(CVM_TET#2,S13) /1/: .0078
Y(CVM_TET#2,S14) /1/: .0078
Y(CVM_TET#2,S21) /1/: .168
Y(CVM_TET#2,S22) /1/: .168
Y(CVM_TET#2,S23) /1/: .168
Y(CVM_TET#2,S24) /1/: .0012
Y(CVM_TET#2,S25) /1/: .0012
Y(CVM_TET#2,S26) /1/: .0012
Y(CVM_TET#2,S31) /1/: 5e-6
Y(CVM_TET#2,S32) /1/: .002
Y(CVM_TET#2,S33) /1/: .002
Y(CVM_TET#2,S34) /1/: .002
Y(CVM_TET#2,S4) /1/: 1e-6
POLY_3:
POLY_3: s-s-c cvm#3 *
... the command in full is SET_START_CONSTITUTION
POLY_3:
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Global equilibrium calculation turned off, you can turn it on with
ADVANCED_OPTIONS GLOBAL_MINIMIZATION Y,,,,,,,,,
19 ITS, CPU TIME USED 0 SECONDS
POLY_3: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VMCS/: 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 1.000000E+00, Mass in grams 1.000000E+01
Total Gibbs energy -3.10213E+03, Enthalpy -2.96850E+03, Volume 0.000000E+00

Component      Moles      M-Fraction  Activity   Potential  Ref.stat
A                6.0000E-01  6.0000E-01  2.0465E-02 -1.9401E+03 SER
B                4.0000E-01  4.0000E-01  6.0538E-05 -4.8452E+03 SER

CVM_TET          Status ENTERED      Driving force 0.0000E+00
Moles 5.6950E-01, Mass 5.6950E+00, Volume fraction 0.0000E+00 Mole fractions:
A 5.89207E-01 B 4.10793E-01
Constitution:
S25 5.78440E-01 S23 1.28068E-02 S33 4.13398E-03 S22 2.56479E-04
S14 1.76120E-01 S21 1.28068E-02 S0 3.76373E-03 S32 1.15932E-04
S12 1.76120E-01 S24 1.28068E-02 S13 2.78465E-03 S34 1.15932E-04
S26 1.28068E-02 S31 4.13398E-03 S11 2.78465E-03 S4 3.67798E-06

CVM_TET#2        Status ENTERED      Driving force 0.0000E+00
Moles 4.3050E-01, Mass 4.3050E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.14278E-01 B 3.85722E-01
Constitution:
S11 4.21306E-01 S14 1.38900E-02 S33 4.69234E-03 S25 3.19866E-03
S23 1.69717E-01 S13 1.38900E-02 S34 4.69234E-03 S24 3.19866E-03
S21 1.69717E-01 S12 1.38900E-02 S0 4.13973E-03 S31 5.05554E-05
S22 1.69717E-01 S32 4.69234E-03 S26 3.19866E-03 S4 8.90403E-06

CVM_TET#3        Status ENTERED      Driving force -1.0709E-01
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.09450E-01 B 3.90550E-01
Constitution:
S14 1.09230E-01 S23 8.47466E-02 S21 8.47466E-02 S33 8.87560E-03
S13 1.09230E-01 S26 8.47466E-02 S22 8.47466E-02 S34 8.87560E-03
S12 1.09230E-01 S25 8.47466E-02 S0 1.86436E-02 S31 8.87560E-03
S11 1.09230E-01 S24 8.47466E-02 S32 8.87560E-03 S4 4.53364E-04
POLY_3:Hit RETURN to continue
POLY_3: s-c t=40
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
18 ITS, CPU TIME USED 0 SECONDS
POLY_3: s-s-c cvm#3 *
... the command in full is SET_START_CONSTITUTION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
18 ITS, CPU TIME USED 0 SECONDS
POLY_3: L-E
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VXNP/:
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=40, P=1E5, N=1, X(B)=0.4
DEGREES OF FREEDOM 0

Temperature 40.00 K ( -233.15 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 1.000000E+01
Total Gibbs energy -3.06232E+03, Enthalpy -2.98938E+03, Volume 0.000000E+00

Component      Moles      M-Fraction  Activity   Potential  Ref.stat
A                6.0000E-01  6.0000E-01  4.1519E-03 -1.8239E+03 SER
B                4.0000E-01  4.0000E-01  3.7621E-07 -4.9199E+03 SER

CVM_TET          Status ENTERED      Driving force 0.0000E+00
Moles 6.6953E-01, Mass 6.6953E+00, Volume fraction 0.0000E+00 Mole fractions:
A 5.88358E-01 B 4.11642E-01
Constitution:
S25 6.26368E-01 S24 4.57470E-03 S33 6.44301E-04 S22 1.02379E-05

```

```

S14 1.76201E-01 S23 4.57470E-03 S31 6.44301E-04 S34 4.02672E-06
S12 1.76201E-01 S21 4.57470E-03 S13 4.60814E-04 S32 4.02672E-06
S26 4.57470E-03 S0 7.03194E-04 S11 4.60814E-04 S4 2.24689E-08

CVM_TET#2 Status ENTERED Driving force 0.0000E+00
Moles 3.3047E-01, Mass 3.3047E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.23586E-01 B 3.76414E-01
Constitution:
S11 4.81572E-01 S14 4.56422E-03 S32 7.57611E-04 S26 4.03145E-04
S21 1.66859E-01 S12 4.56422E-03 S34 7.57611E-04 S24 4.03145E-04
S23 1.66859E-01 S13 4.56422E-03 S0 6.77145E-04 S31 4.66624E-07
S22 1.66859E-01 S33 7.57611E-04 S25 4.03145E-04 S4 4.50770E-08

CVM_TET#3 Status ENTERED Driving force -3.4466E-01
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.15550E-01 B 3.84450E-01
Constitution:
S11 1.12327E-01 S21 8.23389E-02 S25 8.23389E-02 S33 8.17828E-03
S13 1.12327E-01 S22 8.23389E-02 S24 8.23389E-02 S34 8.17828E-03
S14 1.12327E-01 S23 8.23389E-02 S0 2.33728E-02 S31 8.17828E-03
S12 1.12327E-01 S26 8.23389E-02 S32 8.17828E-03 S4 5.71422E-04
POLY_3:Hit RETURN to continue
POLY_3: s-a-v 1 x(b) 0 .5,,
... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 t 0 100,,
... the command in full is SET_AXIS_VARIABLE
POLY_3: save tcex31a y
... the command in full is SAVE_WORKSPACES
POLY_3: map -
Version R mapping is selected

Organizing start points

NO INITIAL EQUILIBRIUM ADDED, TRYING TO FIX ONE
Generating start point 1
Generating start point 2

Phase region boundary 1 at: 4.116E-01 4.000E+01
CVM_TET
** CVM_TET#2
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex31\tcex
31a.POLY3
Terminating at diagram limit
CALCULATED 27 EQUILIBRIA

Phase region boundary 2 at: 4.116E-01 4.000E+01
CVM_TET
** CVM_TET#2
CALCULATED 26 EQUILIBRIA

Phase region boundary 2 at: 4.240E-01 8.061E+01
CVM_TET
** CVM_TET#2
CVM_TET#3

Phase region boundary 2 at: 4.147E-01 8.061E+01
** CVM_TET#2
CVM_TET#3
*** SORRY CANNOT CONTINUE *** 4

CALCULATED 95 EQUILIBRIA

Phase region boundary 2 at: 4.240E-01 8.061E+01
CVM_TET
** CVM_TET#3
Terminating at diagram limit
CALCULATED 24 EQUILIBRIA
*** LAST BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex31\tcex
31a.POLY3
CPU time for mapping 0 seconds
POLY_3: po
... the command in full is POST

POLY-3 POSTPROCESSOR VERSION 3.2

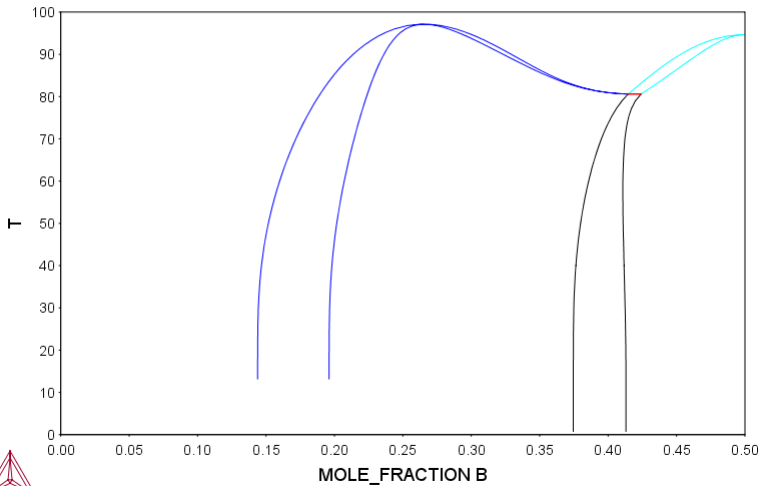
Setting automatic diagram axes

POST: s-d-a x m-f b
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t
... the command in full is SET_DIAGRAM_AXIS
POST: s-s-x n 0 0.5
... the command in full is SET_SCALING_STATUS
POST: s-s-y n 0 100
... the command in full is SET_SCALING_STATUS
POST: set-title example 31a
POST: plot
... the command in full is PLOT_DIAGRAM

```

# example 31a

2016.05.16 14:09:58  
User data 2016.05.16: A, B  
P=1E5, N=1.



```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ Make an experimental data file to overlay the next calculation
POST: make tcex31 y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: back
POLY_3: @@
POLY_3: @@ It is interesting to compare with a CEF without any sro contribution.
POLY_3: @@ This is the classical FCC ordering diagram first calculated
POLY_3: @@ manually by W Shockley, J chem Phys, 6, (1938) p 130
POLY_3: read tcex31a
... the command in full is READ_WORKSPACES
POLY_3: list-ini-eq
... the command in full is LIST_INITIAL_EQUILIBRIA
POLY_3:
POLY_3:
POLY_3:
POLY_3:Hit RETURN to continue
POLY_3: c-st p *=sus
... the command in full is CHANGE_STATUS
POLY_3: c-st p lro lro#2 lro#3=ent 0
... the command in full is CHANGE_STATUS
POLY_3: s-c t=70 x(b)=.4
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
32 ITS, CPU TIME USED 0 SECONDS
POLY_3: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: User dat
```

Conditions:  
T=70, P=1E5, N=1., X(B)=0.4  
DEGREES OF FREEDOM 0

Temperature 70.00 K ( -203.15 C), Pressure 1.000000E+05  
Number of moles of components 1.00000E+00, Mass in grams 1.00000E+01  
Total Gibbs energy -3.08055E+03, Enthalpy -2.95310E+03, Volume 0.00000E+00

Component	Moles	M-Fraction	Activity	Potential	Ref.stat
A	6.0000E-01	6.0000E-01	4.7333E-02	-1.7755E+03	SER
B	4.0000E-01	4.0000E-01	1.7400E-04	-5.0382E+03	SER

LRO ORD Status ENTERED Driving force 0.0000E+00  
Moles 2.6762E-01, Mass 2.6762E+00, Volume fraction 0.0000E+00 Mole fractions:  
A 6.74559E-01 B 3.25441E-01  
Constitution:  
Sublattice 1, Number of sites 2.5000E-01  
A 8.99309E-01 B 1.00691E-01  
Sublattice 2, Number of sites 2.5000E-01  
A 8.99309E-01 B 1.00691E-01  
Sublattice 3, Number of sites 2.5000E-01  
A 8.99309E-01 B 1.00691E-01  
Sublattice 4, Number of sites 2.5000E-01  
B 9.99692E-01 A 3.08116E-04

LRO#2 DISORD Status ENTERED Driving force -4.6485E-01  
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mole fractions:  
A 6.45965E-01 B 3.54035E-01  
Constitution:  
Sublattice 1, Number of sites 2.5000E-01  
A 6.45965E-01 B 3.54035E-01  
Sublattice 2, Number of sites 2.5000E-01  
A 6.45965E-01 B 3.54035E-01  
Sublattice 3, Number of sites 2.5000E-01  
A 6.45965E-01 B 3.54035E-01  
Sublattice 4, Number of sites 2.5000E-01  
A 6.45965E-01 B 3.54035E-01

LRO#3 ORD Status ENTERED Driving force 0.0000E+00  
Moles 7.3238E-01, Mass 7.3238E+00, Volume fraction 0.0000E+00 Mole fractions:  
A 5.72756E-01 B 4.27244E-01  
Constitution:  
Sublattice 1, Number of sites 2.5000E-01  
A 9.99661E-01 B 3.38612E-04  
Sublattice 2, Number of sites 2.5000E-01  
A 9.99661E-01 B 3.38612E-04  
Sublattice 3, Number of sites 2.5000E-01  
B 8.54150E-01 A 1.45850E-01  
Sublattice 4, Number of sites 2.5000E-01

```

B 8.54150E-01 A 1.45850E-01
POLY_3:Hit RETURN to continue
POLY_3: s-s-c lro#3
... the command in full is SET_START_CONSTITUTION
Y(LRO#3,A) /.9996613878/:
Y(LRO#3,B) /3.386121641E-04/:
Y(LRO#3,A#2) /.9996613878/:
Y(LRO#3,B#2) /3.386121641E-04/:
Y(LRO#3,A#3) /.1458499446/: 0.0001
Y(LRO#3,B#3) /.8541500554/: 0.9999
Y(LRO#3,A#4) /.1458499446/: .6
Y(LRO#3,B#4) /.8541500554/: .4
POLY_3: c-e
... the command in full is COMPUTE EQUILIBRIUM
23 ITS, CPU TIME USED 0 SECONDS
POLY_3: l-e,,,,,
... the command in full is LIST EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=70, P=1E5, N=1., X(B)=0.4
DEGREES OF FREEDOM 0

Temperature 70.00 K ( -203.15 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 1.00000E+01
Total Gibbs energy -3.09267E+03, Enthalpy -2.98506E+03, Volume 0.00000E+00

Component      Moles      M-Fraction Activity Potential Ref.stat
A                6.0000E-01  6.0000E-01 4.1721E-02 -1.8489E+03 SER
B                4.0000E-01  4.0000E-01 1.9961E-04 -4.9583E+03 SER

LRO              ORD      Status ENTERED Driving force -3.9691E-02
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.68667E-01 B 3.31333E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 8.91453E-01 B 1.08547E-01
Sublattice 2, Number of sites 2.5000E-01
A 8.91453E-01 B 1.08547E-01
Sublattice 3, Number of sites 2.5000E-01
A 8.91453E-01 B 1.08547E-01
Sublattice 4, Number of sites 2.5000E-01
B 9.99690E-01 A 3.09926E-04

LRO#2            DISORD Status ENTERED Driving force -4.9687E-01
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.39146E-01 B 3.60854E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 6.39146E-01 B 3.60854E-01
Sublattice 2, Number of sites 2.5000E-01
A 6.39146E-01 B 3.60854E-01
Sublattice 3, Number of sites 2.5000E-01
A 6.39146E-01 B 3.60854E-01
Sublattice 4, Number of sites 2.5000E-01
A 6.39146E-01 B 3.60854E-01

LRO#3            ORD      Status ENTERED Driving force 0.0000E+00
Moles 1.0000E+00, Mass 1.0000E+01, Volume fraction 0.0000E+00 Mole fractions:
A 6.00000E-01 B 4.00000E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 9.98449E-01 B 1.55066E-03
Sublattice 2, Number of sites 2.5000E-01
A 9.98449E-01 B 1.55066E-03
Sublattice 3, Number of sites 2.5000E-01
B 9.92271E-01 A 7.72920E-03
Sublattice 4, Number of sites 2.5000E-01
B 6.04628E-01 A 3.95372E-01
POLY_3:Hit RETURN to continue
POLY_3: s-c x(b)=.33
... the command in full is SET_CONDITION
POLY_3: s-s-c lro *
... the command in full is SET_START_CONSTITUTION
POLY_3: c-e
... the command in full is COMPUTE EQUILIBRIUM
23 ITS, CPU TIME USED 0 SECONDS
POLY_3: l-e,,,,,
... the command in full is LIST EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=70, P=1E5, N=1., X(B)=0.33
DEGREES OF FREEDOM 0

Temperature 70.00 K ( -203.15 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 1.00000E+01
Total Gibbs energy -2.85605E+03, Enthalpy -2.74060E+03, Volume 0.00000E+00

Component      Moles      M-Fraction Activity Potential Ref.stat
A                6.7000E-01  6.7000E-01 5.7336E-02 -1.6639E+03 SER
B                3.3000E-01  3.3000E-01 1.1554E-04 -5.2765E+03 SER

LRO              ORD      Status ENTERED Driving force 0.0000E+00
Moles 7.8876E-02, Mass 7.8876E-01, Volume fraction 0.0000E+00 Mole fractions:
A 6.87496E-01 B 3.12504E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 9.16558E-01 B 8.34422E-02
Sublattice 2, Number of sites 2.5000E-01
A 9.16558E-01 B 8.34422E-02
Sublattice 3, Number of sites 2.5000E-01
A 9.16558E-01 B 8.34422E-02
Sublattice 4, Number of sites 2.5000E-01
B 9.99689E-01 A 3.11152E-04

LRO#2            DISORD Status ENTERED Driving force -4.8130E-01
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.61498E-01 B 3.38502E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 6.61498E-01 B 3.38502E-01
Sublattice 2, Number of sites 2.5000E-01
A 6.61498E-01 B 3.38502E-01
Sublattice 3, Number of sites 2.5000E-01

```

```

A 6.61498E-01 B 3.38502E-01
Sublattice 4, Number of sites 2.5000E-01
A 6.61498E-01 B 3.38502E-01

LRO#3          ORD      Status ENTERED   Driving force 0.0000E+00
Moles 9.2112E-01, Mass 9.2112E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.68502E-01 B 3.31498E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 9.82295E-01 B 1.77045E-02
Sublattice 2, Number of sites 2.5000E-01
A 9.82295E-01 B 1.77045E-02
Sublattice 3, Number of sites 2.5000E-01
B 9.99255E-01 A 7.44800E-04
Sublattice 4, Number of sites 2.5000E-01
A 7.08671E-01 B 2.91329E-01
POLY_3:Hit RETURN to continue
POLY_3: s-a-v 2 t 0 250 5
... the command in full is SET_AXIS_VARIABLE
POLY_3:
POLY_3: list-ini-eq
... the command in full is LIST_INITIAL_EQUILIBRIA
POLY_3:
POLY_3:
POLY_3:Hit RETURN to continue
POLY_3: save tcex31c y
... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3: add -1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3:
POLY_3: list-ini-eq
... the command in full is LIST_INITIAL_EQUILIBRIA
No 1 -1 T=70, P=100000, N=1., X(B)=0.33
POLY_3:
POLY_3:
POLY_3:Hit RETURN to continue
POLY_3: map -
Version R mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2

Phase region boundary 1 at: 3.315E-01 7.000E+01
** LRO
LRO#3
*** SORRY CANNOT CONTINUE *** 4

CALCULATED 41 EQUILIBRIA

Phase region boundary 2 at: 3.315E-01 7.000E+01
** LRO
LRO#3
Terminating at diagram limit
CALCULATED 68 EQUILIBRIA
*** LAST BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex31\tcex
31c.POLY3
CPU time for mapping 1 seconds
POLY_3: @@ Add the A2/L1_2 line
POLY_3: read tcex31c
... the command in full is READ_WORKSPACES
POLY_3:
POLY_3:
POLY_3: list-ini-eq
... the command in full is LIST_INITIAL_EQUILIBRIA
POLY_3:
POLY_3:
POLY_3:
POLY_3: s-c x(b)=.15 t=110
... the command in full is SET_CONDITION
POLY_3: s-a-s f
... the command in full is SET_ALL_START_VALUES
Forcing automatic start values
Automatic start values will be set
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
38 ITS, CPU TIME USED 0 SECONDS
POLY_3: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=110, P=1E5, N=1., X(B)=0.15
DEGREES OF FREEDOM 0

Temperature 110.00 K ( -163.15 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 1.00000E+01
Total Gibbs energy -1.66707E+03, Enthalpy -1.39975E+03, Volume 0.00000E+00

Component      Moles      M-Fraction Activity Potential Ref.stat
A                8.5000E-01 8.5000E-01 7.3635E-01 -2.7991E+02 SER
B                1.5000E-01 1.5000E-01 2.9909E-05 -9.5277E+03 SER

LRO          ORD      Status ENTERED   Driving force 0.0000E+00
Moles 7.2552E-01, Mass 7.2552E+00, Volume fraction 0.0000E+00 Mole fractions:
A 8.40743E-01 B 1.59257E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 9.74694E-01 B 2.53056E-02
Sublattice 2, Number of sites 2.5000E-01
A 9.74694E-01 B 2.53056E-02
Sublattice 3, Number of sites 2.5000E-01
A 9.74694E-01 B 2.53056E-02
Sublattice 4, Number of sites 2.5000E-01
B 5.61112E-01 A 4.38888E-01

LRO#2          DISORD Status ENTERED   Driving force -8.1131E-02
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mole fractions:

```

```

A 8.60606E-01 B 1.39394E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 8.60606E-01 B 1.39394E-01
Sublattice 2, Number of sites 2.5000E-01
A 8.60606E-01 B 1.39394E-01
Sublattice 3, Number of sites 2.5000E-01
A 8.60606E-01 B 1.39394E-01
Sublattice 4, Number of sites 2.5000E-01
A 8.60606E-01 B 1.39394E-01

LRO#3 DISORD Status ENTERED Driving force 0.0000E+00
Moles 2.7448E-01, Mass 2.7448E+00, Volume fraction 0.0000E+00 Mole fractions:
A 8.74469E-01 B 1.25531E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 8.74469E-01 B 1.25531E-01
Sublattice 2, Number of sites 2.5000E-01
A 8.74469E-01 B 1.25531E-01
Sublattice 3, Number of sites 2.5000E-01
A 8.74469E-01 B 1.25531E-01
Sublattice 4, Number of sites 2.5000E-01
A 8.74469E-01 B 1.25531E-01
POLY_3:Hit RETURN to continue
POLY_3:
POLY_3: list-ini-eq
... the command in full is LIST_INITIAL_EQUILIBRIA
POLY_3:
POLY_3:
POLY_3:Hit RETURN to continue
POLY_3: map -
Version R mapping is selected

Organizing start points

NO INITIAL EQUILIBRIUM ADDED, TRYING TO FIX ONE
Generating start point 1
Generating start point 2

Phase region boundary 1 at: 1.593E-01 1.100E+02
LRO
** LRO#3
MAPPING TERMINATED 1
CALCULATED 55 EQUILIBRIA

Phase region boundary 2 at: 1.593E-01 1.100E+02
LRO
** LRO#3
Terminating at diagram limit
CALCULATED 69 EQUILIBRIA
*** LAST BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex31\tcex
31c.POLY3
CPU time for mapping 0 seconds
POLY_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

```

```

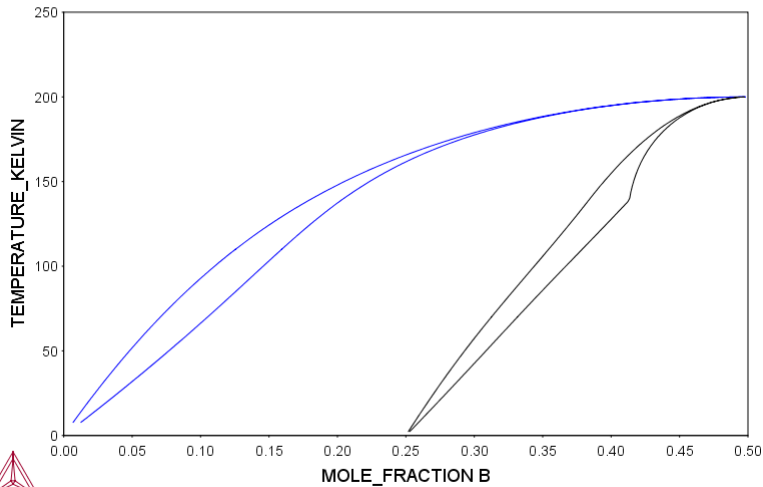
Setting automatic diagram axes

POST: s-s x n 0.5
... the command in full is SET_SCALING_STATUS
POST: @@ Usually some 2nd order lines also appear
POST: set-title example 31b
POST:
POST: plot
... the command in full is PLOT DIAGRAM

```

**example 31b**

2016.05.16.14.09.59  
User data 2016.05.16: A,B  
P=1E5, N=1.



```

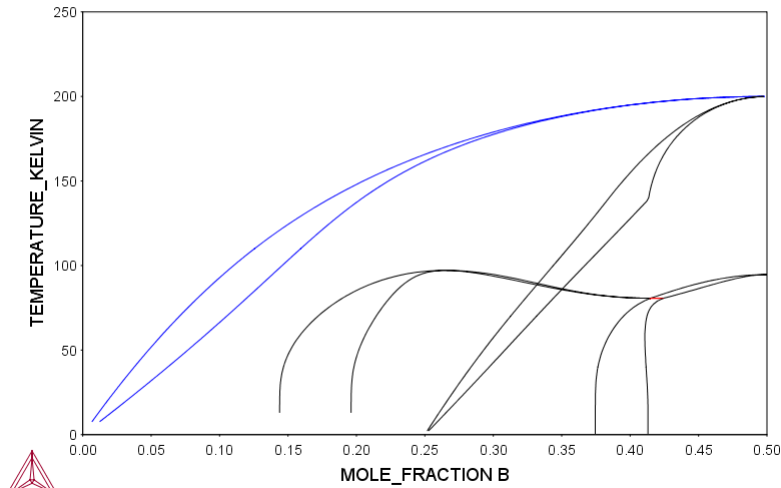
POST:
POST:
POST:Hit RETURN to continue
POST: a-e-d y tcex31 0; 1;
... the command in full is APPEND_EXPERIMENTAL_DATA
POST:
POST: set-title example 31c
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```



# example 31c

2016.05.16 14:09:59  
User data 2016.05.16: A, B  
P=1E5, N=1.



```
POST:
POST:Hit RETURN to continue
POST: ba
... the command in full is BACK
POLY_3: read tcex31c
... the command in full is READ_WORKSPACES
POLY_3: go g
... the command in full is GOTO_MODULE
GIBBS ENERGY SYSTEM version 5.2
GES: @@ Now we will add a reciprocal parameter to LRO which describes
GES: @@ the SRO contribution. The default value of this is
GES: @@ the bond energy. One can have 3 different such parameters
GES: @@ depending on if one is at 25%B, 50%B or 75%B. Here we just take the
GES: @@ same value.
GES:
GES: e-sym f GSROAA,,UIJ;,,,,
... the command in full is ENTER_SYMBOL
GES: e-sym f GSROAB,,UIJ;,,,,
... the command in full is ENTER_SYMBOL
GES: e-sym f GSROBB,,UIJ;,,,,
... the command in full is ENTER_SYMBOL
GES:
GES: e-par l(lro,a,b:a,b:*),,,GSROAB;,,,,
... the command in full is ENTER_PARAMETER
L(LRO,A,B:A,B:*;0)
GES: e-par l(lro,a,b:*:a,b*),,,GSROAB;,,,,
... the command in full is ENTER_PARAMETER
L(LRO,A,B:*:A,B;*;0)
GES: e-par l(lro,a,b:*:a,b),,,GSROAB;,,,,
... the command in full is ENTER_PARAMETER
L(LRO,A,B:*:A,B;0)
GES: e-par l(lro,*:a,b:a,b*),,,GSROAB;,,,,
... the command in full is ENTER_PARAMETER
L(LRO,*:A,B:A,B;*;0)
GES: e-par l(lro,*:a,b:*:a,b),,,GSROAB;,,,,
... the command in full is ENTER_PARAMETER
L(LRO,*:A,B:*:A,B;0)
GES: e-par l(lro,*:a,b:a,b),,,GSROAB;,,,,
... the command in full is ENTER_PARAMETER
L(LRO,*:A,B:A,B;0)
GES: l-p-d lro
... the command in full is LIST_PHASE_DATA

LRO
$ THIS PHASE HAS A DISORDERED CONTRIBUTION FROM FCC_A1
EXCESS MODEL IS REDLICH-KISTER MUGGIANU
4 SUBLATTICES, SITES .25: .25: .25: .25
CONSTITUENTS: A,B : A,B : A,B : A,B

G(LRO,A:A:A;0) = 0.0
G(LRO,B:A:A;0) = +GA3B1
G(LRO,A:B:A;0) = +GA3B1
G(LRO,B:B:A;0) = +GA2B2
G(LRO,A:A:B;0) = +GA3B1
G(LRO,B:A:B;0) = +GA2B2
G(LRO,A:B:B;0) = +GA2B2
G(LRO,B:B:B;0) = +GA1B3
G(LRO,A:A:B;0) = +GA3B1
G(LRO,B:A:B;0) = +GA2B2
G(LRO,A:B:B;0) = +GA2B2
G(LRO,B:B:B;0) = +GA1B3
G(LRO,A:A:B;0) = +GA2B2
G(LRO,B:A:B;0) = +GA1B3
G(LRO,A:B:B;0) = +GA1B3
G(LRO,B:B:B;0) = 0.0
L(LRO,A,B:A,B:*;0) = +GSROAB
L(LRO,A,B:*:A,B;*;0) = +GSROAB
L(LRO,A,B:*:A,B;0) = +GSROAB
L(LRO,*:A,B:A,B;*;0) = +GSROAB
L(LRO,*:A,B:*:A,B;0) = +GSROAB
L(LRO,*:A,B:A,B;0) = +GSROAB

GES:
GES:Hit RETURN to continue
GES: @@ These reciprocal parameters do not give any contribution to the
GES: @@ disordered state as the contribution from the ordered phase is zero there.
GES: @@ But it is in the disordered state that the sro contribution
GES: @@ to the Gibbs energy is most important. We must add regular solution
GES: @@ parameters to the FCC phase giving the same contribution. These can
GES: @@ be derived by setting all site-fractions for the same element equal,
GES: @@ i.e. the disordered state.
```

```

GES: e-par 1(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 1(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 1(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 1(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 1(fcc,a,b;4),,-0.375*GSROAA+0.75*GSROAB-0.375*GSROBB;,,,,,
... the command in full is ENTER_PARAMETER
L(FCC_A1,A,B;4)
GES: l-p-d fcc
... the command in full is LIST_PHASE_DATA

FCC_A1
$ THIS PHASE IS THE DISORDERED PART OF LRO
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
CONSTITUENTS: A,B

G(FCC_A1,A;0)-G(FCC,A;0) = 0.0
G(FCC_A1,B;0)-G(FCC,B;0) = 0.0
L(FCC_A1,A,B;0) = +GA3B1+1.5*GA2B2+GA1B3+.375*GSROAA+.75*GSROAB
+.375*GSROBB
L(FCC_A1,A,B;1) = +2*GA3B1-2*GA1B3+.75*GSROAA-.75*GSROBB
L(FCC_A1,A,B;2) = +GA3B1-1.5*GA2B2+GA1B3-1.5*GSROAB
L(FCC_A1,A,B;3) = -.75*GSROAA+.75*GSROBB
L(FCC_A1,A,B;4) = -.375*GSROAA+.75*GSROAB-.375*GSROBB

GES:
GES:Hit RETURN to continue
GES: ba
... the command in full is BACK
POLY_3: c-st p lro#3=e 0
... the command in full is CHANGE_STATUS
POLY_3: l-c
... the command in full is LIST_CONDITIONS
T=70, P=1E5, N=1., X(B)=0.33
DEGREES OF FREEDOM 0
POLY_3:
POLY_3: s-c t=40
... the command in full is SET_CONDITION
POLY_3: s-a-s f
... the command in full is SET_ALL_START_VALUES
Forcing automatic start values
Automatic start values will be set
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Global equilibrium calculation turned off, you can turn it on with
ADVANCED_OPTIONS GLOBAL_MINIMIZATION Y,,,,,,,,,
27 ITS, CPU TIME USED 0 SECONDS
POLY_3: l-e,,,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=40, P=1E5, N=1., X(B)=0.33
DEGREES OF FREEDOM 0

Temperature 40.00 K ( -233.15 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 1.000000E+01
Total Gibbs energy -2.81177E+03, Enthalpy -2.73484E+03, Volume 0.000000E+00

Component      Moles      M-Fraction  Activity   Potential  Ref.stat
A                6.7000E-01  6.7000E-01  5.5303E-03 -1.7286E+03 SER
B                3.3000E-01  3.3000E-01  2.8612E-07 -5.0109E+03 SER

LRO              ORD      Status ENTERED  Driving force 0.0000E+00
Moles 9.1974E-01, Mass 9.1974E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.79151E-01 B 3.20849E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 9.05532E-01 B 9.44682E-02
Sublattice 2, Number of sites 2.5000E-01
A 9.05532E-01 B 9.44682E-02
Sublattice 3, Number of sites 2.5000E-01
A 9.05532E-01 B 9.44682E-02
Sublattice 4, Number of sites 2.5000E-01
B 9.99993E-01 A 6.81574E-06

LRO#2            DISORD Status ENTERED  Driving force -3.8166E-01
Moles 0.0000E+00, Mass 0.0000E+00, Volume fraction 0.0000E+00 Mole fractions:
A 6.26318E-01 B 3.73682E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 6.26318E-01 B 3.73682E-01
Sublattice 2, Number of sites 2.5000E-01
A 6.26318E-01 B 3.73682E-01
Sublattice 3, Number of sites 2.5000E-01
A 6.26318E-01 B 3.73682E-01
Sublattice 4, Number of sites 2.5000E-01
A 6.26318E-01 B 3.73682E-01

LRO#3            ORD      Status ENTERED  Driving force 0.0000E+00
Moles 8.0263E-02, Mass 8.0263E-01, Volume fraction 0.0000E+00 Mole fractions:
A 5.65144E-01 B 4.34856E-01
Constitution:
Sublattice 1, Number of sites 2.5000E-01
A 9.99996E-01 B 4.15407E-06
Sublattice 2, Number of sites 2.5000E-01
A 9.99996E-01 B 4.15407E-06
Sublattice 3, Number of sites 2.5000E-01
B 8.69708E-01 A 1.30292E-01
Sublattice 4, Number of sites 2.5000E-01
B 8.69708E-01 A 1.30292E-01
POLY_3:Hit RETURN to continue
POLY_3: save tcex3ld y
... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3: list-ini-eq
... the command in full is LIST_INITIAL_EQUILIBRIA

```

```

POLY_3:
POLY_3:
POLY_3:Hit RETURN to continue
POLY_3: map -
Version R mapping is selected

Organizing start points

NO INITIAL EQUILIBRIUM ADDED, TRYING TO FIX ONE
Generating start point  1
Generating start point  2

Phase region boundary  1 at:  3.208E-01  4.000E+01
LRO
** LRO#3
TOO LONG JUMP IN AXIS, SKIPPING NODE
MAPPING TERMINATED 1
CALCULATED  30 EQUILIBRIA

Phase region boundary  2 at:  3.208E-01  4.000E+01
LRO
** LRO#3
CALCULATED  22 EQUILIBRIA

Phase region boundary  2 at:  3.685E-01  7.734E+01
LRO
LRO#2
** LRO#3

Phase region boundary  2 at:  4.193E-01  7.734E+01
** LRO#2
LRO#3
Terminating at diagram limit
CALCULATED  23 EQUILIBRIA

Phase region boundary  2 at:  3.685E-01  7.734E+01
LRO
** LRO#2
Terminating at diagram limit
CALCULATED  88 EQUILIBRIA
*** LAST BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex31\tcex
31d.POLY3
CPU time for mapping 0 seconds
POLY_3: post

```

POLY-3 POSTPROCESSOR VERSION 3.2

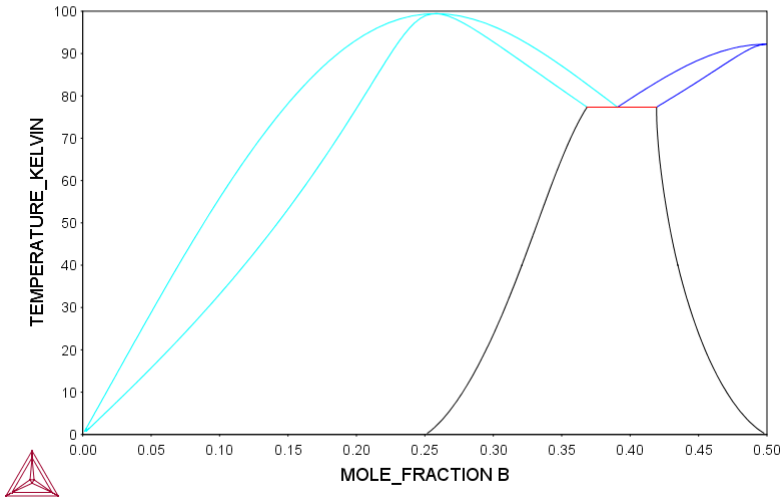
Setting automatic diagram axes

```

POST: set-title example 31d
POST: s-s y n
... the command in full is SET_SCALING_STATUS
MIN VALUE : 0 100
POST:
POST: plot
... the command in full is PLOT DIAGRAM
example 31d

2016.05.16:14:10.00
User data 2016.05.16: A, B
P=1E5, N=1.

```



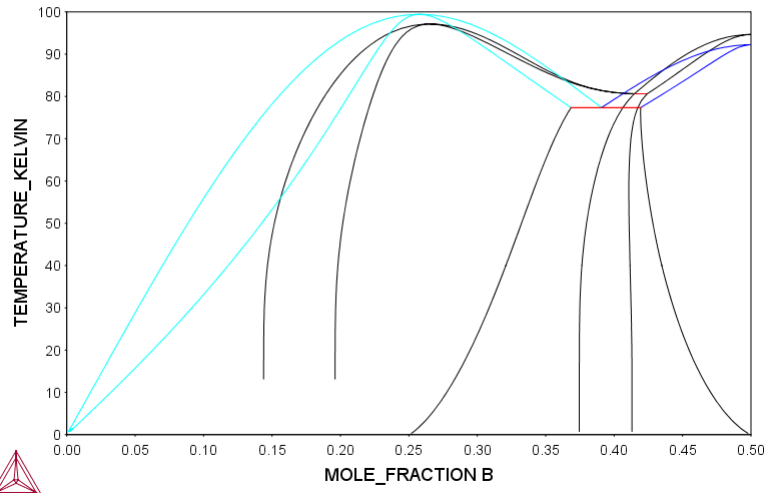
```

POST:
POST:Hit RETURN to continue
POST: a-e-d y tcex31 0; 1;
... the command in full is APPEND_EXPERIMENTAL_DATA
POST: set-title example 31e
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

### example 31e

2016.05.16 14:10:00  
User data 2016.05.16: A, B  
P=1E5, N=1.



POST:  
POST: set-inter  
... the command in full is SET\_INTERACTIVE\_MODE  
POST:

AboutMACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex32\tcex32.TCM"SYS: set-echo

```
SYS: @@
SYS: @@
SYS: @@ Calculation of oxide layers on steel
SYS: @@ and show how to append databases
SYS: @@
SYS: set-log ex32,,,
SYS: go da
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
L12_FCC          B2_BCC          B2_VACANCY
HIGH_SIGMA      DICTRA_FCC_A1 REJECTED
TDB_TCFE8: sw tcf7
... the command in full is SWITCH_DATABASE
Current database: Steels/Fe-Alloys v7.0

VA DEFINED
L12_FCC          B2_BCC          B2_VACANCY
HIGH_SIGMA      DICTRA_FCC_A1 REJECTED
TDB_TCFE7: d-sys fe cr c v mn si
... the command in full is DEFINE_SYSTEM
FE              CR              C
V               MN              SI
DEFINED
TDB_TCFE7: rej ph /all
... the command in full is REJECT
GAS:G           LIQUID:L        BCC_A2
FCC_A1          HCP_A3          DIAMOND_FCC_A4
GRAPHITE        CEMENTITE      M23C6
M7C3            M5C2            M3C2
MC_ETa          KSI_CARBIIDE    A1_KAPPA
KAPPA           Z_PHASE         FE4N_LP1
FECN_CHI        SIGMA          CHI_A12
LAVES_PHASE_C14 M3SI          G_PHASE
CR3SI           FE2SI          MSI
M5SI3           AL4C3          FE8SI2C
SIC REJECTED
TDB_TCFE7: rest ph fcc_a1 bcc_a2 hcp_a3 m23 m7 cementite
... the command in full is RESTORE
FCC_A1          BCC_A2          HCP_A3
M23C6           M7C3            CEMENTITE
RESTORED
TDB_TCFE7: get
... the command in full is GET_DATA
REINITIATING GES5 .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....
```

#### List of references for assessed data

'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'  
 'J-O. Andersson, Calphad, 11 (1987), 271-276; TRITA 0314; C-CR'  
 'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'  
 'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C-  
 -FE'  
 'W. Huang, Metall. Trans. A, 21A (1990), 2115-2123; TRITA-MAC 411 (Rev  
 1989); C-FE-MN'  
 'J. Lacaze and B. Sundman, Metall. Mater. Trans. A, 22A (1991), 2211-2223;  
 Fe-Si and Fe-Si-C'  
 'W. Huang, TRITA-MAC 431 (1990); C-V'  
 'J-O. Andersson and B. Sundman, Calphad, 11 (1987), 83-92; TRITA 0270  
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 'B.-J. Lee, Metall. Trans. A, 24A (1993), 1919-1933; Cr-Mn, Fe-Cr-Mn'  
 'B.-J. Lee, KRISS, unpublished research, during 1993-1995'  
 'B.-J. Lee, TRITA-MAC 474 (1991); Cr-Fe-V'  
 'W. Huang, Calphad, 13 (1989), 243-252; TRITA-MAC 388 (rev 1989); FE-MN'  
 'W. Huang, TRITA-MAC 432 (Rev 1989,1990); FE-V'  
 'J-O. Andersson, Calphad, 7 (1983), 305-315 (parameters revised 1986 due  
 to new description of V) TRITA 0201 (1982); FE-V'  
 'J.E. Tibballs, SI Norway (1991) Rep. 890221-5; Mn-Si'  
 'W. Huang, TRITA-MAC 439 (1990); Mn-V, Fe-Mn-V \*'  
 'M.H. Rand and N. Saunders, COST 507 Report (1998); Si-V'  
 'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'  
 'J-O. Andersson, Metall. Trans. A, 19A (1988), 627-636 TRITA 0207 (1986);  
 C-CR-FE'  
 'B.-J. Lee, Metall. Trans. A, 24A (1993), 1017-1025; Fe-Cr-Mn-C'  
 'J. Miettinen and B. Hallstedt, Calphad, 22 (1998), 231-256; Fe-Si and Fe  
 -Si-C'  
 'W. Huang, TRITA-MAC 432 (1990); C-Fe-V'  
 'A. Fernandez Guillermet and W. Huang, TRITA-MAC 440 (1990); Mn-V-C \*'  
 'A. Forsberg and J. Agren, J. Phase Equil., 14 (1993), 354-363; Fe-Mn-Si'  
 'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;  
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 M23C6'  
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 'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'  
 'P. Villars and L.D. Calvert (1985). Pearsons handbook of crystallographic  
 data for intermetallic phases. Metals park, Ohio. American Society for  
 Metals; Molar volumes'  
 'C. Qiu, ISIJ International, 32 (1992), 1117-1127; C-Cr-Fe-Mo'  
 'Unassessed parameter'  
 'K. Frisk, Metall. Trans. A, 21A (1990), 2477-2488; TRITA 0409 (1989); CR  
 -FE-N'  
 'K. Frisk, Calphad, 17 (1993), 335-349; Cr-Mn-N'  
 'W. Huang, TRITA-MAC 441 (1990); Fe-Mn-V-C'  
 'P. Gustafson, Metall. Trans. A, 19A (1988), 2547-2554; TRITA-MAC 348,  
 (1987); C-CR-FE-W'  
 'B.-J. Lee, TRITA-MAC 475 (1991); C-Cr-Fe-V'  
 'C. Qiu, Metall. Trans. A, 24A (1993), 2393-2409; Cr-Fe-Mn-N'  
 'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Cementite'

'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; SIGMA and M7C3'  
'Thermo-Calc Software (2008): Volume data updated for TCFE6 database (TCFE  
v6, April, 2008).'  
'A. Fernandez Guillermet and G. Grimvall, J. Phys. Chem. Solids, 1992, Vol.  
53, pp. 105-125; Molar volumes'

-OK-

**TDB\_TCFE7:** @@ All oxides from the substance database

**TDB\_TCFE7:** app ssub5

... the command in full is APPEND\_DATABASE

Current database: SGTE Substances Database v5.1

VA DEFINED

**APP:**

**APP:** d-sys fe cr v si mn o c

... the command in full is DEFINE\_SYSTEM

FE CR V

SI MN O

C DEFINED

**APP:** get

... the command in full is GET\_DATA

ELEMENTS .....

SPECIES .....

PHASES .....

... the command in full is AMEND\_PHASE\_DESCRIPTION

... the command in full is AMEND\_PHASE\_DESCRIPTION

... the command in full is AMEND\_PHASE\_DESCRIPTION

... the command in full is AMEND\_PHASE\_DESCRIPTION

... the command in full is AMEND\_PHASE\_DESCRIPTION

... the command in full is AMEND\_PHASE\_DESCRIPTION

... the command in full is AMEND\_PHASE\_DESCRIPTION

PARAMETERS ...

FUNCTIONS .....

List of references for assessed data

C1<G> T.C.R.A.S. Class: 1

C1<G> C<G>

C101<G> JANAF THERMOCHEMICAL TABLES SGTE \*\*

C101<G> CO<G>

CARBON MONOXIDE <GAS>

STANDARD STATE : CODATA KEY VALUE. /CP FROM JANAF PUB. 9/65

C102<G> T.C.R.A.S. Class: 2

C102<G> CO2<G>

CARBON DIOXIDE <GAS>

C1S11<G> T.C.R.A.S. Class: 5

C1S11<G> SiC<G>

SILICON CARBIDE <GAS>

C1S12<G> T.C.R.A.S. Class: 6

C1S12<G> Si2C<G>

DISILICON CARBIDE <GAS>

C1S13<G> THERMODATA 02/94 BC

C1S13<G> Si3C<G>

C1S14<G> THERMODATA 02/94 BC

C1S14<G> Si4C<G>

C2<G> T.C.R.A.S. Class: 2

C2<G>

CARBON Diatomic Gas.

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C201<G> C2O<G>

C2S11<G> JANAF THERMOCHEMICAL TABLES SGTE \*\*

C2S11<G> SiC2<G>

PUBLISHED BY JANAF AT 3/67

C2S12<G> THERMODATA 02/94 BC

C2S12<G> Si2C2<G>

C2S13<G> THERMODATA 03/94 BC

C2S13<G> Si3C2<G>

C3<G> T.C.R.A.S. Class: 6

C3<G>

CARBON <TRIATOMIC GAS>

C302<G> T.C.R.A.S. Class: 6

C302<G>

C4<G> T.C.R.A.S. Class: 7

C4<G>

C5<G> T.C.R.A.S. Class: 7

C5<G>

C5FE105<G> JANAF 1982 SGTE

C5FE105<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  
60Cg>=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)

CR101<G> T.C.R.A.S. Class: 5

CR101<G> CrO<G>

CR102<G> T.C.R.A.S. Class: 6

CR102<G> CrO2<G>

CHROMIUM DIOXIDE <GAS>

CR103<G> T.C.R.A.S. Class: 6

CR103<G> CrO3<G>

CHROMIUM TRIOXIDE <GAS>

CR2<G> THERMODATA

CR2<G> Cr2<G>

New assessment (H form and S only)

CR201<G> T.C.R.A.S. Class: 6

CR201<G> Cr2O<G>

CR202<G> T.C.R.A.S. Class: 6

CR202<G> Cr2O2<G>

CR203<G> T.C.R.A.S. Class: 7

CR203<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  
FE101<G> TCRAS 5-F FEO IRON OXIDE 23/11/06  
FE101<G> FeO<G>  
FE102<G> T.C.R.A.S Class: 6  
FE102<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  
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MN1<G> Mn<G>  
MANGANESE <GAS>  
28/01/93  
MN101<G> T.C.R.A.S. Class: 2  
MN101<G> MnO<G>  
MANGANESE<2> OXIDE <GAS>  
MN102<G> T.C.R.A.S. Class: 7  
MN102<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>  
O1S11<G> T.C.R.A.S. Class: 1  
O1S11<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.  
O2S11<G> T.C.R.A.S. Class: 5  
O2S11<G> SiO2<G>  
SILICON DIOXIDE <GAS>  
O2S12<G> CHATILLON(1995)  
O2S12<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>  
O2S11<BETA-QUARTZ> N.P.L.  
O2S11\_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  
CO.88V1 THERMODATA 01/93  
CO.88V1 VC0.88  
28/01/93  
CIFE103 N.P.L. SGTE \*\*  
CIFE103 FeCO3 Siderite  
IRON<2> CARBONATE  
DECOMPOSES BEFORE FUSION.  
CIFE3 N.P.L. SGTE \*\*  
CIFE3 Fe3C Cementite  
CEMENTITE  
CIMN103 KUBASCHEWSKI EVANS ALCOCK 1967 SGTE \*\*  
CIMN103 MnCO3  
MANGANESE<2> CARBONATE  
CIMN3 M. ANCEY, Y. DENIEL SGTE  
CIMN3 Mn3C  
TRIMANGANESE MONOCARBIDE  
C1S11<C1S11\_ALPHA> JANAF THERMOCHEMICAL TABLES SGTE \*\*  
C1S11\_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.  
C1S11<C1S11\_BETA> JANAF THERMOCHEMICAL TABLES SGTE  
C1S11\_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  
REASSESSMENT BY B.URHENIUS  
C5FE105<L> I. BARIN 3rd. Edition

C5FE105\_Liquid Fe(CO)<sub>5</sub>\_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<sup>-1</sup> 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<sup>-1</sup>.  
 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).  
 C6CR106 I. BARIN 3rd. Edition  
 C6CR106 Cr(CO)<sub>6</sub>  
 CHROMIUM HEXACARBONYL  
 SUBLIMATION AT 424K.  
 C6CR23 JANAF THERMOCHEMICAL TABLES SGTE  
 C6CR23 Cr<sub>2</sub>3C<sub>6</sub>  
 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 Mn<sub>2</sub>3C<sub>6</sub>  
 CR102 S.G.T.E. SGTE \*\*  
 CR102 CrO<sub>2</sub>  
 CHROMIUM DIOXIDE  
 O.KUBASCHEWSKI'S REASSESSMENT 1979  
 CR103 S.G.T.E. SGTE \*\*  
 CR103 CrO<sub>3</sub>  
 CHROMIUM TRIOXIDE  
 O.KUBASCHEWSKI'S REASSESSMENT 1979  
 CR1S11 T.C.R.A.S. Class: 6  
 CR1S11 CrSi  
 CHROMIUM SILICON  
 CR1S12 T.C.R.A.S. Class: 7  
 CR1S12 CrSi<sub>2</sub>  
 CHROMIUM 2-SILICON  
 CR2FE104 KUBASCHEWSKI EVANS ALCOCK 1967 SGTE  
 CR2FE104 FeCr<sub>2</sub>O<sub>4</sub> FeO-Cr<sub>2</sub>O<sub>3</sub>  
 DELTAH 298 CALCULATED FROM OXIDES =-13100CAL/MOL(#1000)  
 CR2O3 T.C.R.A.S. Class: 7  
 CR2O3 Cr<sub>2</sub>O<sub>3</sub>  
 CHROMIUM<3> OXIDE  
 cp refitted by AP because of low T FC at 306K  
 CR3S11 T.C.R.A.S. Class: 7  
 CR3S11 Cr<sub>3</sub>Si  
 3-CHROMIUM 2-SILICON  
 CR5O12 S.G.T.E. SGTE \*\*  
 CR5O12 Cr<sub>5</sub>O<sub>12</sub>  
 5-CHROMIUM 12-OXIDE  
 CR5O12: 5-CHROMIUM 12-OXIDE \*\*DECOMPOSITION (643 -->705 K)  
 O.KUBASCHEWSKI'S REASSESSMENT 1979.  
 CR5S13 T.C.R.A.S. Class: 7  
 CR5S13 Cr<sub>5</sub>Si<sub>3</sub>  
 5-CHROMIUM 3-SILICON  
 CR8O21 S.G.T.E. SGTE \*\*  
 CR8O21 Cr<sub>8</sub>O<sub>21</sub>  
 8-CHROMIUM 21-OXIDE  
 O.KUBASCHEWSKI'S REASSESSMENT 1971  
 CR8O21 8-CHROMIUM 21-OXIDE, DECOMPOSITION (600 --> 640K.)  
 O2S11<CRISTOBALITE> N.P.L.  
 O2S11\_CRISTOBALITE SiO<sub>2</sub>\_CRISTOBALITE  
 Data from an assessment by T I Barry, reported in paper on CaO-SiO<sub>2</sub>  
 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)  
 FE2O4S11<FAYALITE> S.G.T.E.  
 FE2O4S11 Fe<sub>2</sub>SiO<sub>4</sub> FAYALITE 2FeO-SiO<sub>2</sub>  
 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  
 FE1O3S11 THERMODATA 01/93  
 FE1O3S11 FeSiO<sub>3</sub> FeO-SiO<sub>2</sub>  
 28/01/93  
 FE1O4V2 THERMODATA 01/93  
 FE1O4V2 FeV<sub>2</sub>O<sub>4</sub> FeO-V<sub>2</sub>O<sub>3</sub>  
 28/01/93  
 FE1O6V2 THERMODATA 01/93  
 FE1O6V2 FeV<sub>2</sub>O<sub>6</sub> FeO-V<sub>2</sub>O<sub>5</sub>  
 IRON VANADATE  
 28/01/93 Td = 1023 K.  
 FE1S11 THERMODATA 01/93  
 FE1S11 FeSi  
 IRON SILICIDE  
 28/01/93  
 FE1S12.33 THERMODATA 01/93  
 FE1S12.33 FeSi<sub>2</sub>.33  
 LEBOITE <ALPHA>  
 28/01/93 LEBOITE (ALPHA).  
 FE1S12 THERMODATA 01/93  
 FE1S12 FeSi<sub>2</sub>  
 LEBOITE <BETA>  
 28/01/93 LEBOITE (BETA). Td = 1243K  
 FE2MN1O4 O. KUBASCHEWSKI DCS REPORT 7 . SGTE  
 FE2MN1O4 MnFe<sub>2</sub>O<sub>4</sub> MnO-Fe<sub>2</sub>O<sub>3</sub>  
 MANGANESE DIIRON TETRAOXIDE  
 BARIN  
 KNACKE ED 73 REF \*,5,1 (KUBASCHEWSKI) .  
 FE2O3<FE2O3\_GAMMA> T.C.R.A.S. Class: 5  
 FE2O3\_GAMMA Fe<sub>2</sub>O<sub>3</sub>\_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 MN01.5-1.6. 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
FE0.94701<WUSTITE> T.C.R.A.S Class: 5
FE0.94701 Fe0.9470 WUSTITE
WUSTITE. Data provided by T.C.R.A.S. in 2000
20080222 AAZ TCRAS2006 : dH, S

```

-OK-

APP: go p-3  
... the command in full is GOTO\_MODULE

POLY version 3.32

POLY\_3:

POLY\_3: s-c b(cr)=16 b(v)=.1 b(c)=1 b(mn)=.3 b(si)=.3 t=1073 p=1e5 b=100  
... the command in full is SET\_CONDITION

```

POLY_3: l-c
... the command in full is LIST_CONDITIONS
B(CR)=16, B(V)=0.1, B(C)=1, B(MN)=0.3, B(SI)=0.3, T=1073, P=1E5, B=100
DEGREES OF FREEDOM 1
POLY_3:
POLY_3: @@set-start-value y(fcc_a1#2,si)=1e-2
POLY_3: @@set-start-value y(fcc_a1#1,si)=1e-12
POLY_3: set-start-const fcc#1
... the command in full is SET_START_CONSTITUTION
Y(FCC_A1,CR) /1/: 1e-6
Y(FCC_A1,FE) /1/: 0.999
Y(FCC_A1,MN) /1/: 4e-6
Y(FCC_A1,SI) /1/: 1e-9
Y(FCC_A1,V) /1/: 5e-7
Y(FCC_A1,C#2) /1/: 4e-2
Y(FCC_A1,VA#2) /1/: 0.96
POLY_3: set-start-const fcc#2
... the command in full is SET_START_CONSTITUTION
Y(FCC_A1#2,CR) /1/: 2e-2
Y(FCC_A1#2,FE) /1/: 0.4
Y(FCC_A1#2,MN) /1/: 7e-4
Y(FCC_A1#2,SI) /1/: 4e-4
Y(FCC_A1#2,V) /1/: 0.6
Y(FCC_A1#2,C#2) /1/: 0.8
Y(FCC_A1#2,VA#2) /1/: 0.2
POLY_3:Hit RETURN to continue
POLY_3: @@ We have atomic oxygen as component, later we will use
POLY_3: @@ the partial pressure of o2 as output. The state variable LNACR is
POLY_3: @@ the chemical potential divided by RT, usual values are between -40 and 0
POLY_3: s-c lnacr(o)=-27
... the command in full is SET_CONDITION
POLY_3: s-r-s o gas * 1e5
... the command in full is SET_REFERENCE_STATE
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 9034 grid points in 0 s
135 ITS, CPU TIME USED 0 SECONDS
POLY_3: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VMCS/: VMCS
Output from POLY-3, equilibrium = 1, label A0 , database: SSUB5

Conditions:
B(CR)=16, B(V)=0.1, B(C)=1, B(MN)=0.3, B(SI)=0.3, T=1073, P=1E5, B=100,
LNACR(O)=-27
DEGREES OF FREEDOM 0

Temperature 1073.00 K ( 799.85 C), Pressure 1.000000E+05
Number of moles of components 2.23269E+00, Mass in grams 1.00000E+02
Total Gibbs energy -2.78602E+05, Enthalpy -1.28388E+05, Volume 9.84603E-06

Component      Moles      W-Fraction Activity Potential Ref.stat
C               8.3257E-02  1.0000E-02  1.9687E-01 -1.4499E+04 SER
CR              3.0772E-01  1.6000E-01  5.3299E-06 -1.0833E+05 SER
FE              1.3332E+00  7.4453E-01  4.8257E-03 -4.7585E+04 SER
MN              5.4607E-03  3.0000E-03  1.0592E-07 -1.4328E+05 SER
O               4.9044E-01  7.8466E-02  1.8795E-12 -2.4088E+05 GAS
SI              1.0681E-02  3.0000E-03  7.4765E-14 -2.6965E+05 SER
V               1.9631E-03  1.0000E-03  2.9371E-08 -1.5473E+05 SER

FCC_A1          Status ENTERED      Driving force 0.0000E+00
Moles 1.3878E+00, Mass 7.5134E+01, Volume fraction 1.0000E+00 Mass fractions:
FE 9.90936E-01 CR 3.05125E-04 V 6.34556E-05 O 0.00000E+00
C 8.62498E-03 MN 7.05949E-05 SI 1.76803E-07

CR2O3_S         Status ENTERED      Driving force 0.0000E+00
Moles 7.6819E-01, Mass 2.3351E+01, Volume fraction 0.0000E+00 Mass fractions:
CR 6.84207E-01 C 0.00000E+00 MN 0.00000E+00 V 0.00000E+00
O 3.15793E-01 SI 0.00000E+00 FE 0.00000E+00

TEPHROITE       Status ENTERED      Driving force 0.0000E+00
Moles 1.8775E-02, Mass 5.4167E-01, Volume fraction 0.0000E+00 Mass fractions:
MN 5.44054E-01 SI 1.39069E-01 V 0.00000E+00 CR 0.00000E+00
O 3.16878E-01 C 0.00000E+00 FE 0.00000E+00

BETA_QUARTZ      Status ENTERED      Driving force 0.0000E+00
Moles 2.3997E-02, Mass 4.8061E-01, Volume fraction 0.0000E+00 Mass fractions:
O 5.32554E-01 C 0.00000E+00 MN 0.00000E+00 CR 0.00000E+00
SI 4.67446E-01 V 0.00000E+00 FE 0.00000E+00

GRAPHITE         Status ENTERED      Driving force 0.0000E+00
Moles 2.9304E-02, Mass 3.5197E-01, Volume fraction 0.0000E+00 Mass fractions:
C 1.00000E+00 SI 0.00000E+00 MN 0.00000E+00 CR 0.00000E+00
V 0.00000E+00 O 0.00000E+00 FE 0.00000E+00

O3V2_S          Status ENTERED      Driving force 0.0000E+00
Moles 4.6737E-03, Mass 1.4010E-01, Volume fraction 0.0000E+00 Mass fractions:
V 6.79762E-01 C 0.00000E+00 MN 0.00000E+00 CR 0.00000E+00
O 3.20238E-01 SI 0.00000E+00 FE 0.00000E+00
POLY_3: sh lnacr(o)
... the command in full is SHOW_VALUE
LNACR(O)=-27
POLY_3: @@ List also the activity of O2
POLY_3: show lnacr(o2,gas)
... the command in full is SHOW_VALUE
LNACR(O2,GAS)=-54
POLY_3:Hit RETURN to continue
POLY_3: @@ Vary the normalized chemical potential of oxygen between -20 and -40
POLY_3: s-a-v 1 lnacr(o)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: -40
Max value /1/: -20
Increment /.5/: 0.25
POLY_3: save tcex32 y
... the command in full is SAVE_WORKSPACES
POLY_3: step
... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: NORMAL
No initial equilibrium, using default
Step will start from axis value -27.0000
...OK

```

Phase Region from -27.0000 for:  
 BETA\_QUARTZ  
 CR2O3\_S  
 FCC\_A1  
 GRAPHITE  
 O3V2\_S  
 TEPHROITE  
 Global check of adding phase at -2.66392E+01  
 Calculated 4 equilibria

Phase Region from -26.6392 for:  
 BETA\_QUARTZ  
 CR2FE1O4\_S  
 CR2O3\_S  
 FCC\_A1  
 GRAPHITE  
 O3V2\_S  
 TEPHROITE  
 Calculated 2 equilibria

Phase Region from -26.6392 for:  
 BETA\_QUARTZ  
 CR2FE1O4\_S  
 FCC\_A1  
 GRAPHITE  
 O3V2\_S  
 TEPHROITE  
 Global check of adding phase at -2.48680E+01  
 Calculated 10 equilibria

Phase Region from -24.8680 for:  
 BETA\_QUARTZ  
 CR2FE1O4\_S  
 FCC\_A1  
 FE1O4V2\_S  
 GRAPHITE  
 O3V2\_S  
 TEPHROITE  
 Calculated 2 equilibria

Phase Region from -24.8680 for:  
 BETA\_QUARTZ  
 CR2FE1O4\_S  
 FCC\_A1  
 FE1O4V2\_S  
 GRAPHITE  
 TEPHROITE  
 Global check of adding phase at -2.32956E+01  
 Calculated 9 equilibria

Phase Region from -23.2956 for:  
 GAS  
 BETA\_QUARTZ  
 CR2FE1O4\_S  
 FCC\_A1  
 FE1O4V2\_S  
 GRAPHITE  
 TEPHROITE  
 Calculated 2 equilibria

Phase Region from -23.2956 for:  
 GAS  
 BETA\_QUARTZ  
 CR2FE1O4\_S  
 FCC\_A1  
 FE1O4V2\_S  
 TEPHROITE  
 Global check of adding phase at -2.30914E+01  
 Calculated 4 equilibria

Phase Region from -23.0914 for:  
 GAS  
 BETA\_QUARTZ  
 CR2FE1O4\_S  
 FAYALITE  
 FCC\_A1  
 FE1O4V2\_S  
 TEPHROITE  
 Calculated 2 equilibria

Phase Region from -23.0914 for:  
 GAS  
 CR2FE1O4\_S  
 FAYALITE  
 FCC\_A1  
 FE1O4V2\_S  
 TEPHROITE  
 Global check of adding phase at -2.28036E+01  
 Calculated 4 equilibria

Phase Region from -22.8036 for:  
 GAS  
 CR2FE1O4\_S  
 FAYALITE  
 FCC\_A1  
 FE1O1\_S  
 FE1O4V2\_S  
 TEPHROITE  
 Calculated 2 equilibria

Phase Region from -22.8036 for:  
 GAS  
 CR2FE1O4\_S  
 FAYALITE  
 FE1O1\_S  
 FE1O4V2\_S  
 TEPHROITE  
 Global test at -2.10000E+01 .... OK  
 Terminating at -20.0000  
 Calculated 15 equilibria

Phase Region from -27.0000 for:  
 BETA\_QUARTZ  
 CR2O3\_S  
 FCC\_A1

```

GRAPHITE
O3V2_S
TEPHROITE
Global check of adding phase at -2.78680E+01
Calculated      6 equilibria

Phase Region from  -27.8680      for:
BETA_QUARTZ
CR2O3_S
FCC_A1
FCC_A1#2
GRAPHITE
O3V2_S
TEPHROITE
Calculated      2 equilibria

Phase Region from  -27.8680      for:
BETA_QUARTZ
CR2O3_S
FCC_A1
FCC_A1#2
GRAPHITE
TEPHROITE
Global check of adding phase at -2.82727E+01
Calculated      5 equilibria

Phase Region from  -28.2727      for:
BETA_QUARTZ
CEMENTITE
CR2O3_S
FCC_A1
FCC_A1#2
GRAPHITE
TEPHROITE
Calculated      2 equilibria

Phase Region from  -28.2727      for:
BETA_QUARTZ
CEMENTITE
CR2O3_S
FCC_A1
FCC_A1#2
TEPHROITE
Global check of adding phase at -2.95967E+01
Calculated      8 equilibria

Phase Region from  -29.5967      for:
BETA_QUARTZ
CEMENTITE
CR2O3_S
FCC_A1
FCC_A1#2
M7C3
TEPHROITE
Calculated      2 equilibria

Phase Region from  -29.5967      for:
BETA_QUARTZ
CEMENTITE
CR2O3_S
FCC_A1
M7C3
TEPHROITE
Global check of removing phase at -2.96631E+01
Calculated      3 equilibria

Phase Region from  -29.6631      for:
BETA_QUARTZ
CR2O3_S
FCC_A1
M7C3
TEPHROITE
Global check of adding phase at -3.04150E+01
Calculated      6 equilibria

Phase Region from  -30.4150      for:
BCC_A2
BETA_QUARTZ
CR2O3_S
FCC_A1
M7C3
TEPHROITE
Global check of removing phase at -3.04211E+01
Calculated      3 equilibria

Phase Region from  -30.4211      for:
BCC_A2
BETA_QUARTZ
CR2O3_S
M7C3
TEPHROITE
Global check of removing phase at -3.10968E+01
Calculated      6 equilibria

Phase Region from  -31.0968      for:
BCC_A2
BETA_QUARTZ
M7C3
TEPHROITE
Global check of removing phase at -3.12857E+01
Calculated      4 equilibria

Phase Region from  -31.2857      for:
BCC_A2
M7C3
TEPHROITE
Global check of removing phase at -3.14255E+01
Calculated      3 equilibria

Phase Region from  -31.4255      for:
BCC_A2
M7C3
Global test at -3.32500E+01 .... OK
Global test at -3.57500E+01 .... OK
Global test at -3.82500E+01 .... OK
Terminating at  -40.0000

```

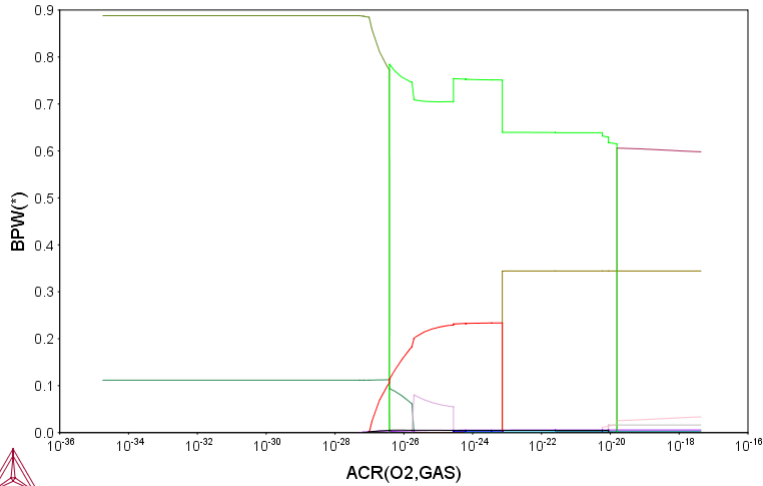
Calculated 38 equilibria  
 \*\*\* Buffer saved on file:  
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex32\tcex32.POLY3

POLY\_3:  
 POLY\_3: po  
 ... the command in full is POST  
 POLY-3 POSTPROCESSOR VERSION 3.2

POST:  
 POST: s-d-a x acr(o2,gas)  
 ... the command in full is SET\_DIAGRAM\_AXIS  
 POST: s-d-a y bpw(\*)  
 ... the command in full is SET\_DIAGRAM\_AXIS  
 COLUMN NUMBER /\*/: \*  
 POST: s-a-ty  
 ... the command in full is SET\_AXIS\_TYPE  
 AXIS (X, Y OR Z) : x  
 AXIS TYPE /LINEAR/: log  
 POST: set-title example 32a  
 POST: plot  
 ... the command in full is PLOT DIAGRAM

example 32a

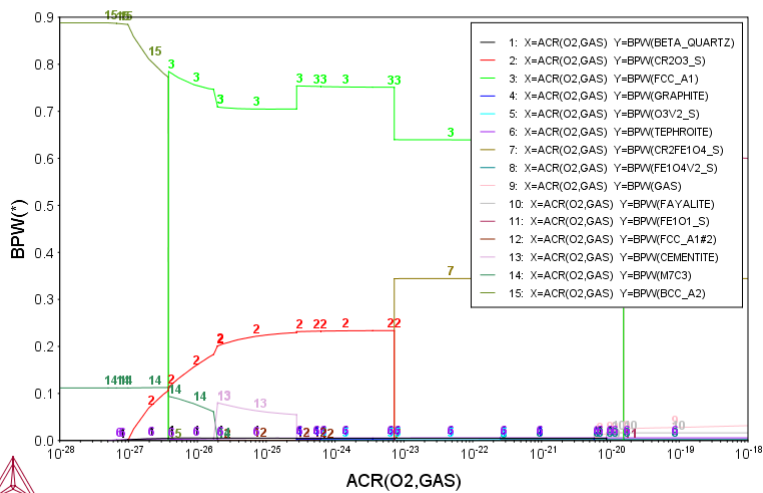
2016.05.16.14.12.13  
 SSUBS: C, CR, FE, MN, O, SI, V  
 B(CR)=16., B(V)=0.1, B(C)=1., B(MN)=0.3, B(SI)=0.3, T=1073, P=1E5, B=100.



POST:  
 POST:Hit RETURN to continue  
 POST: s-lab f  
 ... the command in full is SET\_LABEL\_CURVE\_OPTION  
 POST: s-s x n 1e-28 1e-18  
 ... the command in full is SET\_SCALING\_STATUS  
 POST: set-title example 32b  
 POST:  
 POST: plot  
 ... the command in full is PLOT DIAGRAM

example 32b

2016.05.16.14.12.14  
 SSUBS: C, CR, FE, MN, O, SI, V  
 B(CR)=16., B(V)=0.1, B(C)=1., B(MN)=0.3, B(SI)=0.3, T=1073, P=1E5, B=100.



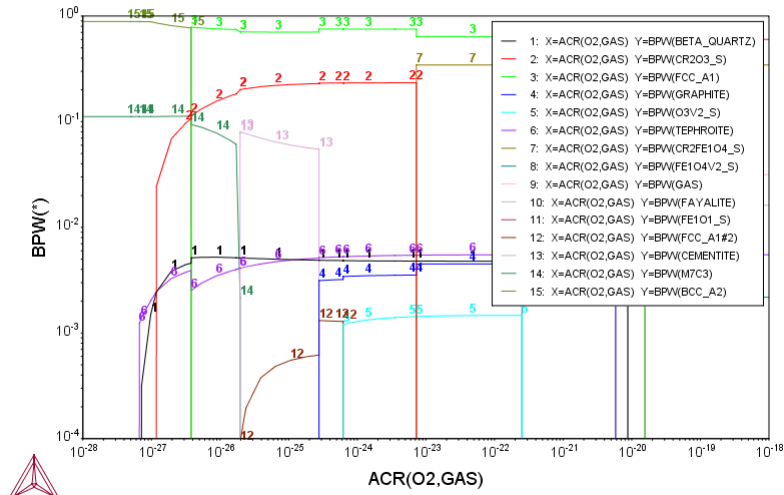
POST:  
 POST:Hit RETURN to continue  
 POST: s-a-ty y  
 ... the command in full is SET\_AXIS\_TYPE  
 AXIS TYPE /LINEAR/: log  
 POST: s-s y n 1e-4 1  
 ... the command in full is SET\_SCALING\_STATUS  
 POST: set-title example 32c  
 POST:  
 POST: plot  
 ... the command in full is PLOT DIAGRAM

### example 32c

2016.05.16.14.12.16

SSUBS: C, CR, FE, MN, O, SI, V

B(CR)=16., B(V)=0.1, B(C)=1., B(MN)=0.3, B(SI)=0.3, T=1073, P=1E5, B=100.



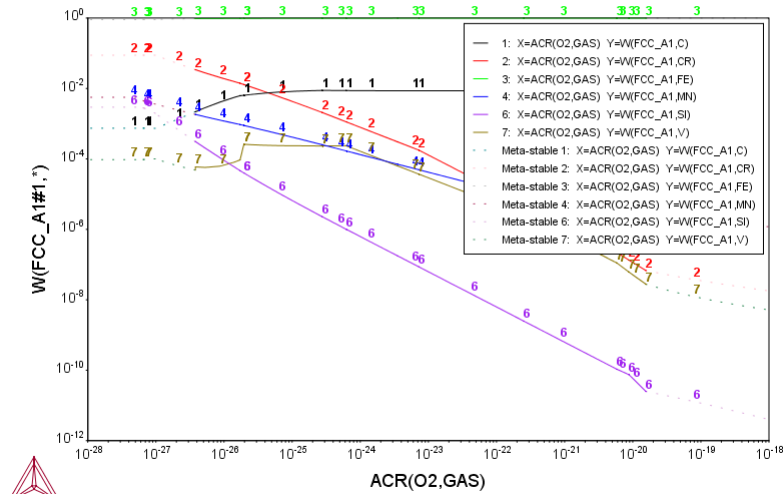
```
POST:
POST:Hit RETURN to continue
POST: @@ Finally plot how the composition of FCC varies.
POST: s-d-a y w(fcc_a1#1,*)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: s-s y n 1e-12 1
... the command in full is SET_SCALING_STATUS
POST: set-title example 32d
POST:
POST: plot
... the command in full is PLOT DIAGRAM
```

### example 32d

2016.05.16.14.12.17

SSUBS: C, CR, FE, MN, O, SI, V

B(CR)=16., B(V)=0.1, B(C)=1., B(MN)=0.3, B(SI)=0.3, T=1073, P=1E5, B=100.



```
POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:
```

## tcex33

### About

Software (build 9533) running on WinNT 64-bit wordlength  
Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118  
License library version: 8.5.1.0017  
Linked: Mon May 16 09:31:44 2016

```
SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex33\tcex33.TCM"SYS: set-echo
```

```
SYS: @@
```

```
SYS: @@
```

```
SYS: @@ Benchmark calculation for Fe-Cr-C isopleth
```

```
SYS: @@
```

```
SYS: set-log ex33,,,,
```

```
SYS: go da
```

```
... the command in full is GOTO_MODULE
```

```
THERMODYNAMIC DATABASE module
```

```
Current database: Steels/Fe-Alloys v8.0
```

```
VA DEFINED
```

```
L12_FCC
```

```
B2_BCC
```

```
B2_VACANCY
```

```
HIGH_SIGMA
```

```
DICTRA_FCC_A1 REJECTED
```

```
TDB_TCFE8: sw FEDEMO
```

```
... the command in full is SWITCH_DATABASE
```

```
Current database: Iron Demo Database
```

```
VA /- DEFINED
```

```
TDB_FEDEMO: d-sys fe cr c
```

```
... the command in full is DEFINE_SYSTEM
```

```
FE CR C
```

```
DEFINED
```

```
TDB_FEDEMO: rej ph /all
```

```
... the command in full is REJECT
```

```
GAS:G LIQUID:L BCC_A2
```

```
CEMENTITE CHI_A12 DIAMOND_FCC_A4
```

```
FCC_A1 GRAPHITE HCP_A3
```

```
KSI_CARBIDE LAVES_PHASE_C14 M23C6
```

```
M3C2 M5C2 M7C3
```

```
SIGMA REJECTED
```

```
TDB_FEDEMO: rest ph liquid fcc_a1 bcc_a2 graphite sigma cementite m23 m7 m3c2
```

```
... the command in full is RESTORE
```

```
LIQUID:L FCC_A1 BCC_A2
```

```
GRAPHITE SIGMA CEMENTITE
```

```
M23C6 M7C3 M3C2
```

```
RESTORED
```

```
TDB_FEDEMO: get
```

```
... the command in full is GET_DATA
```

```
REINITIATING GES5 .....
```

```
ELEMENTS .....
```

```
SPECIES .....
```

```
PHASES .....
```

```
... the command in full is AMEND_PHASE_DESCRIPTION
```

```
... the command in full is AMEND_PHASE_DESCRIPTION
```

```
PARAMETERS ...
```

```
FUNCTIONS ....
```

List of references for assessed data

'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'

'B. Uhrenius (1993-1994), International journal of refractory metals and hard mater, Vol. 12, pp. 121-127; Molar volumes'

'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'

'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89; Molar volumes'

'X.-G. Lu et al. Calphad 29 (2005) 49-55, Fe P-T diagram'

'J.-O. Andersson, Calphad, 11 (1987), 271-276; TRITA 0314; C-CR'

'B.-J. Lee, Calphad (1993); revision of Fe-Cr and Fe-Ni liquid'

'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C

-FE'

'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'

'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo -C, C-Mn'

'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'

'J.-O. Andersson, Metall. Trans. A, 19A (1988), 627-636 TRITA 0207 (1986); C-CR-FE'

'J.-O. Andersson and B. Sundman, Calphad, 11 (1987), 83-92; TRITA 0270

(1986); CR-FE'

'P. Villars and L.D. Calvert (1985). Pearsons handbook of crystallographic

data for intermetallic phases. Metals park, Ohio. American Society for

Metals; Molar volumes'

'J. Bratberg, Z. Metallkd., Vol 96 (2005), 335-344; Fe-Cr-Mo-C'

'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New

Sigma model'

```
-OK-
```

```
TDB_FEDEMO: go p-3
```

```
... the command in full is GOTO_MODULE
```

```
POLY version 3.32
```

```
POLY_3: s-c t=1200,p=1e5,n=1 w(cr)=.13 w(c)=.01
```

```
... the command in full is SET_CONDITION
```

```
POLY_3: c-e
```

```
... the command in full is COMPUTE_EQUILIBRIUM
```

```
Using global minimization procedure
```

```
Calculated 9529 grid points in 0 s
```

```
Found the set of lowest grid points in 0 s
```

```
Calculated POLY solution 0 s, total time 0 s
```

```
POLY_3: s-a-v 1 w(c) 0 .02
```

```
... the command in full is SET_AXIS_VARIABLE
```

```
Increment /5E-04/: 5E-04
```

```
POLY_3: s-a-v 2 t 800 2000
```

```
... the command in full is SET_AXIS_VARIABLE
```

```
Increment /30/: 30
```

```
POLY_3: save tcex33 y
```

```
... the command in full is SAVE_WORKSPACES
```

```
POLY_3: map
```

```
Version S mapping is selected
```

```
Generating start equilibrium 1
```

```
Generating start equilibrium 2
```

```
Generating start equilibrium 3
```

```
Generating start equilibrium 4
```

```
Generating start equilibrium 5
```

```
Generating start equilibrium 6
```

```
Generating start equilibrium 7
```

Generating start equilibrium 8  
Generating start equilibrium 9  
Generating start equilibrium 10  
Generating start equilibrium 11  
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Tie-lines not in the plane of calculation

Generating start point 1  
Generating start point 2  
Generating start point 3  
Generating start point 4  
Generating start point 5  
Generating start point 6  
Generating start point 7  
Generating start point 8  
Generating start point 9  
Generating start point 10

Working hard

Generating start point 11  
Generating start point 12  
Generating start point 13  
Generating start point 14  
Generating start point 15  
Generating start point 16  
Generating start point 17  
Generating start point 18  
Generating start point 19  
Generating start point 20

Working hard

Generating start point 21  
Generating start point 22  
Generating start point 23  
Generating start point 24  
Generating start point 25  
Generating start point 26  
Generating start point 27  
Generating start point 28

Phase region boundary 1 at: 7.207E-03 8.100E+02  
BCC\_A2  
M23C6

\*\* M7C3  
Calculated.. 2 equilibria  
Terminating at axis limit.

Phase region boundary 2 at: 7.259E-03 8.000E+02  
BCC\_A2  
M23C6

\*\* M7C3  
Calculated. 12 equilibria

Phase region boundary 3 at: 3.778E-03 1.096E+03  
BCC\_A2  
\*\* FCC\_A1#2

M23C6  
\*\* M7C3

Phase region boundary 4 at: 3.778E-03 1.096E+03  
BCC\_A2  
\*\* FCC\_A1

M23C6  
Calculated. 9 equilibria

Phase region boundary 5 at: 8.020E-05 1.125E+03  
BCC\_A2  
\*\* FCC\_A1  
\*\* M23C6

Phase region boundary 6 at: 8.020E-05 1.125E+03  
BCC\_A2  
\*\* FCC\_A1  
Calculated 16 equilibria

Phase region boundary 7 at: 8.020E-05 1.125E+03  
BCC\_A2  
\*\* M23C6

Calculated.. 12 equilibria  
Terminating at axis limit.

Phase region boundary 8 at: 8.020E-05 1.125E+03  
BCC\_A2  
FCC\_A1

\*\* M23C6  
Calculated. 4 equilibria

Phase region boundary 9 at: 1.004E-03 1.155E+03  
\*\* BCC\_A2  
FCC\_A1

\*\* M23C6

Phase region boundary 10 at: 1.004E-03 1.155E+03  
FCC\_A1  
\*\* M23C6

Calculated. 5 equilibria

Phase region boundary 11 at: 2.216E-03 1.245E+03  
FCC\_A1  
\*\* M23C6  
\*\* M7C3

Phase region boundary 12 at: 2.216E-03 1.245E+03  
FCC\_A1  
\*\* M23C6  
M7C3

Calculated. 10 equilibria  
Terminating at known equilibrium

Phase region boundary 13 at: 2.216E-03 1.245E+03  
FCC\_A1  
\*\* M7C3

Calculated. 26 equilibria



Phase region boundary 14 at: 1.143E-02 1.569E+03  
 \*\* LIQUID  
 FCC\_A1  
 \*\* M7C3  
 Phase region boundary 15 at: 1.143E-02 1.569E+03  
 LIQUID  
 FCC\_A1  
 \*\* M7C3  
 Calculated.. 19 equilibria  
 Terminating at axis limit.  
 Phase region boundary 16 at: 1.143E-02 1.569E+03  
 \*\* LIQUID  
 FCC\_A1  
 Calculated. 17 equilibria  
 Phase region boundary 17 at: 4.634E-03 1.684E+03  
 \*\* LIQUID  
 \*\* BCC\_A2  
 FCC\_A1  
 Phase region boundary 18 at: 4.634E-03 1.684E+03  
 \*\* LIQUID  
 BCC\_A2  
 FCC\_A1  
 Calculated. 8 equilibria  
 Phase region boundary 19 at: 1.464E-03 1.696E+03  
 \*\* LIQUID  
 BCC\_A2  
 \*\* FCC\_A1  
 Phase region boundary 20 at: 1.464E-03 1.696E+03  
 \*\* LIQUID  
 BCC\_A2  
 Calculated 18 equilibria  
 Phase region boundary 21 at: 1.464E-03 1.696E+03  
 BCC\_A2  
 \*\* FCC\_A1  
 Calculated 27 equilibria  
 Phase region boundary 22 at: 1.464E-03 1.696E+03  
 LIQUID  
 BCC\_A2  
 \*\* FCC\_A1  
 Calculated. 16 equilibria  
 Phase region boundary 23 at: 8.680E-03 1.714E+03  
 LIQUID  
 \*\* BCC\_A2  
 \*\* FCC\_A1  
 Phase region boundary 24 at: 8.680E-03 1.714E+03  
 LIQUID  
 \*\* FCC\_A1  
 Calculated.. 24 equilibria  
 Terminating at axis limit.  
 Phase region boundary 25 at: 8.680E-03 1.714E+03  
 LIQUID  
 \*\* BCC\_A2  
 Calculated 30 equilibria  
 Phase region boundary 26 at: 8.680E-03 1.714E+03  
 LIQUID  
 \*\* BCC\_A2  
 FCC\_A1  
 Calculated. 10 equilibria  
 Terminating at known equilibrium  
 Phase region boundary 27 at: 4.634E-03 1.684E+03  
 \*\* BCC\_A2  
 FCC\_A1  
 Calculated. 19 equilibria  
 Terminating at known equilibrium  
 Phase region boundary 28 at: 1.143E-02 1.569E+03  
 \*\* LIQUID  
 FCC\_A1  
 M7C3  
 Calculated.. 19 equilibria  
 Terminating at axis limit.  
 Phase region boundary 29 at: 2.216E-03 1.245E+03  
 FCC\_A1  
 M23C6  
 \*\* M7C3  
 Calculated. 7 equilibria  
 Terminating at known equilibrium  
 Phase region boundary 30 at: 1.004E-03 1.155E+03  
 \*\* BCC\_A2  
 FCC\_A1  
 M23C6  
 Calculated. 10 equilibria  
 Terminating at known equilibrium  
 Phase region boundary 31 at: 4.772E-03 1.096E+03  
 BCC\_A2  
 \*\* FCC\_A1  
 M7C3  
 Calculated.. 32 equilibria  
 Terminating at axis limit.  
 Phase region boundary 32 at: 5.640E-03 1.096E+03  
 \*\* BCC\_A2  
 FCC\_A1  
 M7C3  
 Calculated.. 30 equilibria  
 Terminating at axis limit.  
 Phase region boundary 33 at: 4.772E-03 1.096E+03  
 BCC\_A2  
 \*\* M23C6

M7C3  
 Calculated.. 15 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 34 at: 7.207E-03 8.100E+02  
 BCC\_A2  
 M23C6  
 \*\* M7C3  
 Calculated. 12 equilibria  
 Terminating at known equilibrium

Phase region boundary 35 at: 5.000E-04 1.121E+03  
 BCC\_A2  
 \*\* FCC\_A1  
 M23C6  
 Calculated. 2 equilibria  
 Terminating at known equilibrium

Phase region boundary 36 at: 5.000E-04 1.121E+03  
 BCC\_A2  
 \*\* FCC\_A1  
 M23C6  
 Calculated. 8 equilibria  
 Terminating at known equilibrium

Phase region boundary 37 at: 6.833E-03 8.723E+02  
 BCC\_A2  
 M23C6  
 \*\* M7C3  
 Calculated. 10 equilibria  
 Terminating at known equilibrium

Phase region boundary 38 at: 6.833E-03 8.723E+02  
 BCC\_A2  
 M23C6  
 \*\* M7C3  
 Calculated.. 5 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 39 at: 1.317E-02 1.082E+03  
 BCC\_A2  
 \*\* FCC\_A1  
 M7C3  
 Calculated. 18 equilibria  
 Terminating at known equilibrium

Phase region boundary 40 at: 1.317E-02 1.082E+03  
 BCC\_A2  
 \*\* FCC\_A1  
 M7C3  
 Calculated.. 15 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 41 at: 1.004E-02 8.100E+02  
 BCC\_A2  
 \*\* M23C6  
 M7C3  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 42 at: 1.004E-02 8.100E+02  
 BCC\_A2  
 \*\* M23C6  
 M7C3  
 Calculated. 15 equilibria  
 Terminating at known equilibrium

Phase region boundary 43 at: 1.950E-02 1.061E+03  
 BCC\_A2  
 \*\* FCC\_A1  
 M7C3  
 Calculated. 31 equilibria  
 Terminating at known equilibrium

Phase region boundary 44 at: 1.950E-02 1.061E+03  
 BCC\_A2  
 \*\* FCC\_A1  
 M7C3  
 Calculated.. 3 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 45 at: 7.664E-04 1.203E+03  
 \*\* BCC\_A2  
 FCC\_A1  
 Calculated. 3 equilibria  
 Terminating at known equilibrium

Phase region boundary 46 at: 7.664E-04 1.203E+03  
 \*\* BCC\_A2  
 FCC\_A1  
 Calculated. 18 equilibria  
 Terminating at known equilibrium

Phase region boundary 47 at: 3.363E-03 1.203E+03  
 FCC\_A1  
 \*\* M23C6  
 M7C3  
 Calculated. 8 equilibria  
 Terminating at known equilibrium

Phase region boundary 48 at: 3.363E-03 1.203E+03  
 FCC\_A1  
 \*\* M23C6  
 M7C3  
 Calculated. 4 equilibria  
 Terminating at known equilibrium

Phase region boundary 49 at: 7.811E-04 1.597E+03  
 BCC\_A2  
 \*\* FCC\_A1  
 Calculated 27 equilibria

```

Phase region boundary 50 at: 7.811E-04 1.597E+03
  BCC_A2
** FCC_A1
Calculated. 5 equilibria
Terminating at known equilibrium

Phase region boundary 51 at: 9.892E-03 1.597E+03
  LIQUID
  FCC_A1
Calculated. 5 equilibria
Terminating at known equilibrium

Phase region boundary 52 at: 9.892E-03 1.597E+03
  LIQUID
  FCC_A1
Calculated. 14 equilibria
Terminating at known equilibrium

Phase region boundary 53 at: 5.000E-04 1.788E+03
  LIQUID
** BCC_A2
Calculated 22 equilibria

Phase region boundary 54 at: 5.000E-04 1.788E+03
  LIQUID
** BCC_A2
Calculated. 18 equilibria
Terminating at known equilibrium

Phase region boundary 55 at: 6.833E-03 1.730E+03
  LIQUID
** BCC_A2
Calculated 26 equilibria

Phase region boundary 56 at: 6.833E-03 1.730E+03
  LIQUID
** BCC_A2
Calculated. 5 equilibria
Terminating at known equilibrium

Phase region boundary 57 at: 1.317E-02 1.691E+03
  LIQUID
** FCC_A1
Calculated. 10 equilibria
Terminating at known equilibrium

Phase region boundary 58 at: 1.317E-02 1.691E+03
  LIQUID
** FCC_A1
Calculated.. 15 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 59 at: 1.950E-02 1.655E+03
  LIQUID
** FCC_A1
Calculated. 23 equilibria
Terminating at known equilibrium

Phase region boundary 60 at: 1.950E-02 1.655E+03
  LIQUID
** FCC_A1
Calculated.. 3 equilibria
Terminating at known equilibrium
Terminating at axis limit.
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex33\tcex
33.POLY3
CPU time for mapping 5 seconds
POLY_3: post

```

POLY-3 POSTPROCESSOR VERSION 3.2

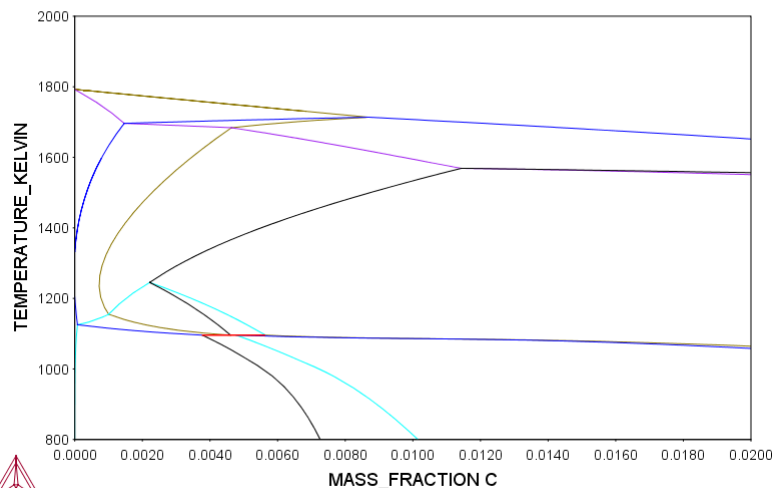
Setting automatic diagram axes

```

POST:
POST: set-title example 33a
POST: plot
... the command in full is PLOT DIAGRAM
                                example 33a

```

2016.05.16.14.14.31  
 FEDEMO: C, CR, FE  
 P=1E5, N=1, W(CR)=0.13



POST:

```
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:
```

**About**

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software (build 9533) running on WinNT 64-bit wordlength  
Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118  
License library version: 8.5.1.0017  
Linked: Mon May 16 09:31:44 2016

**SYS:**SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex34\tcex34.TCM"**SYS:** set-echo

**SYS:** @@

**SYS:** @@ Calculation

**SYS:** @@ of the phase diagram and G curves

**SYS:** @@ in the Al-Zn system

**SYS:** @@

**SYS:** @@ Another example of using the BINARY module

**SYS:** @@

**SYS:** go bin

THERMODYNAMIC DATABASE module

Current database: Steels/Fe-Alloys v8.0

VA DEFINED

L12\_FCC

B2\_BCC

B2\_VACANCY

HIGH\_SIGMA

DICTRA\_FCC\_A1 REJECTED

Simple binary phase diagram calculation module

**Database: /TCBIN/:** TCBIN

Current database: TC Binary Solutions v1.1

VA

/- DEFINED

BCC\_B2

FCC\_L12

FCC\_L102

D021\_HCP REJECTED

**First element:** al zn

**Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase\_Diagram/:** Phase\_Diagram

VA

/- DEFINED

BCC\_B2

FCC\_L12

FCC\_L102

D021\_HCP REJECTED

REINITIATING GES5 .....

AL

ZN DEFINED

GAS:G

LIQUID:L

IONIC\_LIQUID:Y

FCC\_A1

BCC\_A2

A2\_BCC

HCP\_A3

HCP\_ZN

DIAMOND\_A4

BCT\_A5

TETRAGONAL\_A6

RHOMBOHEDRAL\_A7

CBCC\_A12

CUB\_A13

B32\_ALLI

B3\_ZINCBLENDE

C14\_LAVES

C15\_LAVES

C16\_AL2CU

C36\_LAVES

D019\_AL1M3

D513\_AL3NI2

D82\_FEZN\_GAMMA

L10\_ALTI

AGZN\_ZETA

AL5FE4

ALCE\_AMORPHOUS

ALCU\_ETA

FEZN4

FEZN\_DELTA

FEZN\_ZETA REJECTED

LIQUID:L RESTORED

FCC\_A1 RESTORED

HCP\_A3 RESTORED

HCP\_ZN RESTORED

ELEMENTS .....

SPECIES .....

PHASES .....

PARAMETERS ...

FUNCTIONS ....

List of references for assessed data

'A T Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4 p 317-425; '

'A T Dinsdale, SGTE Data for Pure Elements, update 2001'

'S an Mey, Z Metallkde 84(1993)7 p 451-455; Al-Zn'

-OK-

The condition X(ZN)=.1234 created

The condition T=612.43 created

Forcing automatic start values

Automatic start values will be set

Start points provided by database

Version S mapping is selected

Organizing start points

Generating start point 1

Generating start point 2

Phase region boundary 1 at: 5.345E-01 5.000E+02

\*\* FCC\_A1

HCP\_ZN

Calculated.. 10 equilibria

Terminating at axis limit.

Phase region boundary 2 at: 5.027E-01 3.000E+02

\*\* FCC\_A1

HCP\_ZN

Calculated.. 13 equilibria

Phase region boundary 3 at: 5.626E-01 5.504E+02

\*\* FCC\_A1

\*\* FCC\_A1#2

HCP\_ZN

Phase region boundary 4 at: 7.872E-01 5.504E+02

\*\* FCC\_A1

HCP\_ZN

Calculated.. 6 equilibria

Phase region boundary 5 at: 8.211E-01 6.540E+02

\*\* LIQUID

\*\* FCC\_A1

HCP\_ZN

Phase region boundary 6 at: 9.263E-01 6.540E+02

\*\* LIQUID

HCP\_ZN

Calculated 17 equilibria

Phase region boundary 7 at: 7.783E-01 6.540E+02

\*\* LIQUID

FCC\_A1

Calculated 73 equilibria

Phase region boundary 8 at: 3.658E-01 5.504E+02

\*\* FCC\_A1

FCC\_A1#2

Calculated 27 equilibria

Phase region boundary 9 at: 5.345E-01 5.000E+02

\*\* FCC\_A1

HCP\_ZN

Calculated. 5 equilibria

Terminating at known equilibrium

\*\*\* BUFFER SAVED ON FILE:

c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex34\BINARY.POLY3

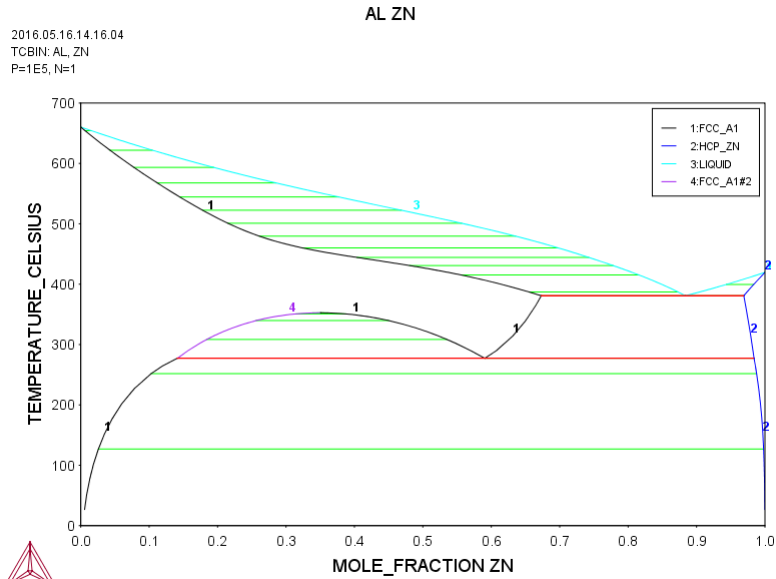
CPU time for mapping 1 seconds

POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

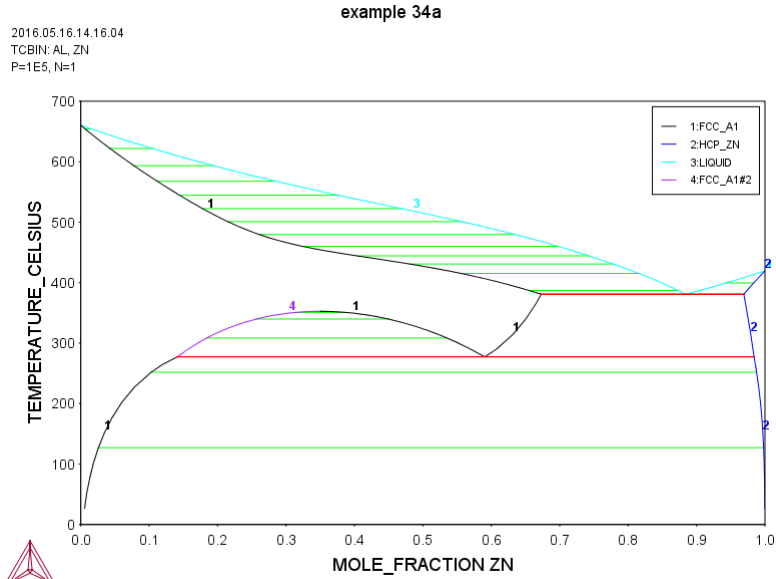
POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes



POST: set-title example 34a

POST: plot



POST:

POST:Hit RETURN to continue

POST: @@ Now plot a G curve at 573 K!

POST: back

Current database: Steels/Fe-Alloys v8.0

VA DEFINED

L12 FCC B2\_BCC B2\_VACANCY

HIGH\_SIGMA DICTRA\_FCC\_A1 REJECTED

SYS: go bin

Current database: Steels/Fe-Alloys v8.0

VA DEFINED

L12\_FCC B2\_BCC B2\_VACANCY

HIGH\_SIGMA                    DICTRA\_FCC\_A1   REJECTED

Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN

Current database: TC Binary Solutions   v1.1

VA                                /-   DEFINED  
BCC\_B2                            FCC\_L12                            FCC\_L102  
D021\_HCP   REJECTED

First element: al zn

Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase\_Diagram/: G

Temperature (C): /1000/: 300

VA                                /-   DEFINED  
BCC\_B2                            FCC\_L12                            FCC\_L102  
D021\_HCP   REJECTED

REINITIATING GES5 .....

AL                                ZN   DEFINED  
GAS:G                            LIQUID:L                            IONIC\_LIQUID:Y  
FCC\_A1                            BCC\_A2                            A2\_BCC  
HCP\_A3                            HCP\_ZN                            DIAMOND\_A4  
BCT\_A5                            TETRAGONAL\_A6                    RHOMBOHEDRAL\_A7  
CBCC\_A12                           CUB\_A13                           B32\_ALLI  
B3\_ZINCBLLENDE                   C14\_LAVES                           C15\_LAVES  
C16\_AL2CU                           C36\_LAVES                           D019\_AL1M3  
D513\_AL3NI2                           D82\_FEZN\_GAMMA                   L10\_ALTI  
AGZN\_ZETA                           AL5FE4                           ALCE\_AMORPHOUS  
ALCU\_ETA                           FEZN4                           FEZN\_DELTA

FEZN\_ZETA   REJECTED

LIQUID:L   RESTORED

FCC\_A1   RESTORED

HCP\_A3   RESTORED

HCP\_ZN   RESTORED

ELEMENTS .....

SPECIES .....

PHASES .....

PARAMETERS ...

FUNCTIONS ....

List of references for assessed data

'A T Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4 p 317-425; '

'A T Dinsdale, SGTE Data for Pure Elements, update 2001'

'S an Mey, Z Metallkde 84(1993)7 p 451-455; Al-Zn'

-OK-

The condition X(ZN)=.1234   created

Forcing automatic start values

Automatic start values will be set

Phase Region from    0.502463        for:

LIQUID  
FCC\_A1  
FCC\_A1#2  
HCP\_A3  
HCP\_ZN

Phase Region from    0.502463        for:

LIQUID  
FCC\_A1  
FCC\_A1#2  
HCP\_A3  
HCP\_ZN

\*\*\* Buffer saved on file \*\*\*

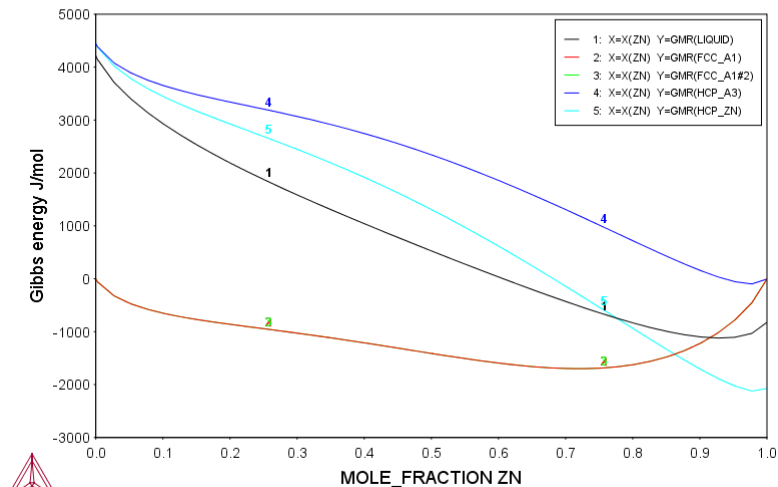
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex34\GCUR

VE.POLY3

POSTPROCESSOR VERSION 3.2

AL ZN

2016.05.16.14.16.11  
TCBIN: AL\_ZN  
P=1E5, N=1, T=573.15



POST: s-s y n -500 1500

POST:

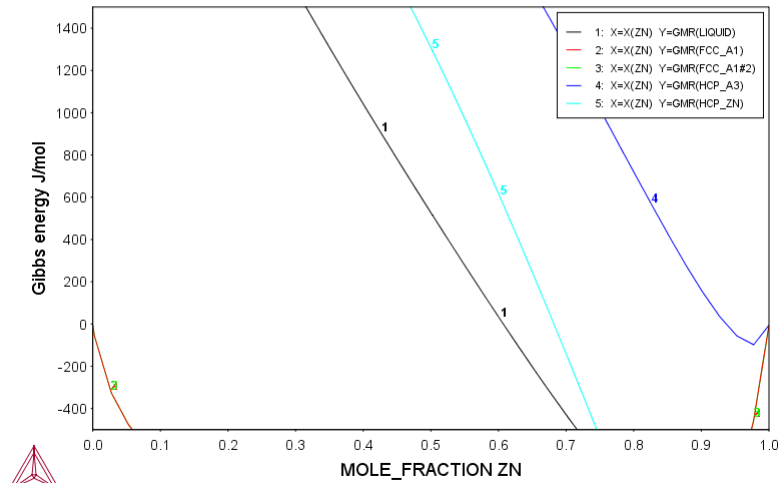
POST: set-title example 34b

POST:

POST: plot

# example 34b

2016.05.16.14.16.11  
TCBIN: AL\_ZN  
P=1E5, N=1, T=573.15



```

POST:
POST:Hit RETURN to continue
POST: @@ Now plot an activity (A) curve at 573 K
POST: back
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
L12_FCC          B2_BCC          B2_VACANCY
HIGH_SIGMA      DICTRA_FCC_A1    REJECTED
SYS: go bin
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
L12_FCC          B2_BCC          B2_VACANCY
HIGH_SIGMA      DICTRA_FCC_A1    REJECTED

Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN
Current database: TC Binary Solutions v1.1

VA          /- DEFINED
BCC_B2      FCC_L12          FCC_L102
D021_HCP    REJECTED

First element: al zn
Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase_Diagram/: A
Temperature (C): /1000/: 300
VA          /- DEFINED
BCC_B2      FCC_L12          FCC_L102
D021_HCP    REJECTED
REINITIATING GES5 .....
AL          ZN DEFINED
GAS:G       LIQUID:L          IONIC_LIQUID:Y
FCC_A1      BCC_A2          A2_BCC
HCP_A3      HCP_ZN          DIAMOND_A4
BCT_A5      TETRAGONAL_A6    RHOMBOHEDRAL_A7
CBCC_A12    CUB_A13          B32_ALLI
B3_ZINCBLLENDE C14_LAVES      C15_LAVES
C16_AL2CU    C36_LAVES      D019_AL1M3
D513_AL3NI2  D82_FEZN_GAMMA    L10_ALTI
AGZN_ZETA    AL5FE4          ALCE_AMORPHOUS
ALCU_ETA     FEZN4           FEZN_DELTA
FEZN_ZETA    REJECTED
LIQUID:L     RESTORED
FCC_A1       RESTORED
HCP_A3       RESTORED
HCP_ZN       RESTORED
ELEMENTS     .....
SPECIES      .....
PHASES       .....
PARAMETERS   ...
FUNCTIONS     ....

List of references for assessed data

'A T Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4 p 317-425; '
'A T Dinsdale, SGTE Data for Pure Elements, update 2001'
'S an Mey, Z Metallkde 84(1993)7 p 451-455; Al-Zn'
-OK-
The condition X(ZN)=.1234 created

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

Forcing automatic start values
Automatic start values will be set
No initial equilibrium, using default
Step will start from axis value 0.123400
...OK

Phase Region from 0.123400 for:
FCC_A1
Global test at 3.23400E-01 .. Backtracking to find phase change for FCC_A1#2
Global test at 1.48400E-01 .... OK
Global check of adding phase at 1.70853E-01
Calculated 5 equilibria

Phase Region from 0.170853 for:
FCC_A1
FCC_A1#2
Global test at 3.48400E-01 .... OK

```



Global check of removing phase at 5.51861E-01  
 Calculated 19 equilibria

Phase Region from 0.551861 for:  
 FCC\_A1#2

Global Check of adding phase at 6.18456E-01  
 Calculated 5 equilibria

Phase Region from 0.618456 for:  
 FCC\_A1#2  
 HCP\_ZN

Global Test at 7.98400E-01 .... OK

Global check of removing phase at 9.81102E-01  
 Calculated 18 equilibria

Phase Region from 0.981102 for:  
 HCP\_ZN

Terminating at 1.00000  
 Calculated 4 equilibria

Phase Region from 0.123400 for:  
 FCC\_A1

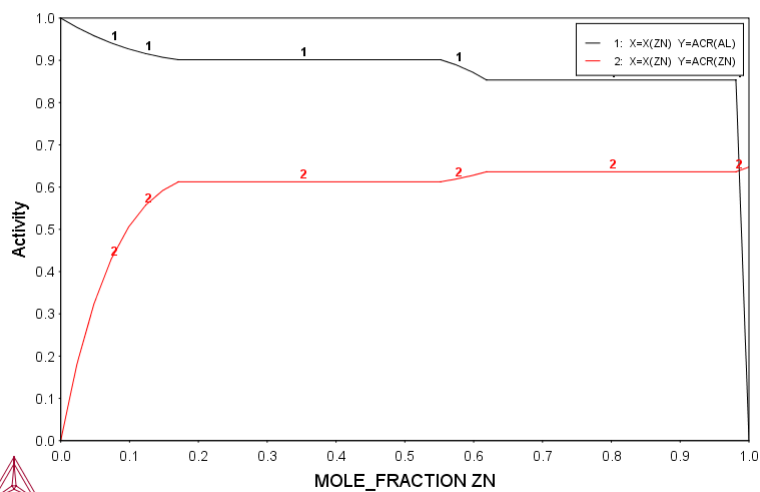
Terminating at 0.100000E-11  
 Calculated 8 equilibria

\*\*\* Buffer saved on file:  
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex34\GCUR  
 VE.POLY3

POSTPROCESSOR VERSION 3.2

### AL ZN

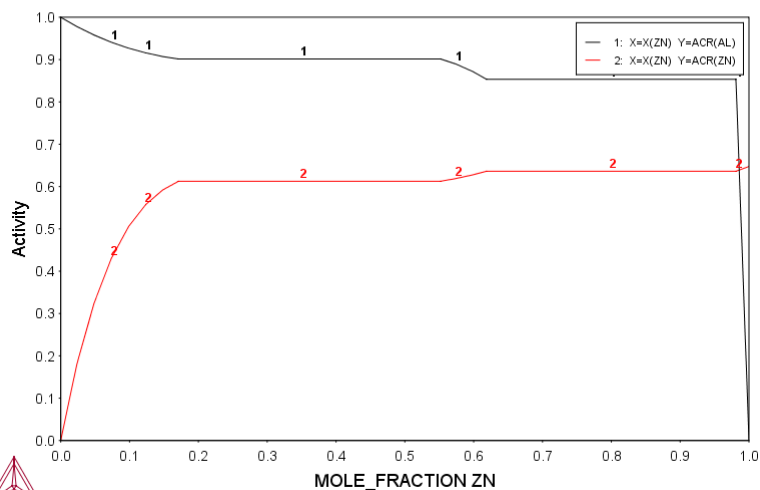
2016.05.16.14.16.17  
 TCBIN: AL\_ZN  
 P=1E5, N=1., T=573.15



POST:  
 POST: set-title example 34c  
 POST:  
 POST: plot

### example 34c

2016.05.16.14.16.18  
 TCBIN: AL\_ZN  
 P=1E5, N=1., T=573.15



POST:  
 POST: Hit RETURN to continue  
 POST: @@ Now plot a Phase fraction (F) curve for x(zn)=.5.  
 POST: @@ The miscibility gap can be found now  
 POST: back  
 Current database: Steels/Fe-Alloys v8.0

VA DEFINED  
 L12\_FCC B2\_BCC B2\_VACANCY  
 HIGH\_SIGMA DICTRA\_FCC\_A1 REJECTED  
 SYS: go bin  
 Current database: Steels/Fe-Alloys v8.0

VA DEFINED  
 L12\_FCC B2\_BCC B2\_VACANCY

HIGH\_SIGMA                    DICTRA\_FCC\_A1   REJECTED

Simple binary phase diagram calculation module

Database: /TCBIN/: TCBIN

Current database: TC Binary Solutions   v1.1

VA                                /-   DEFINED  
BCC\_B2                            FCC\_L12                            FCC\_L102  
D021\_HCP   REJECTED

First element: al zn

Phase Diagram, Phase fraction (F), G- or A-curves (G/A): /Phase\_Diagram/: F

Fraction of: zn /.5/: .5

VA                                /-   DEFINED  
BCC\_B2                            FCC\_L12                            FCC\_L102  
D021\_HCP   REJECTED  
REINITIATING GES5   ....  
AL                                ZN   DEFINED  
GAS:G                            LIQUID:L                            IONIC\_LIQUID:Y  
FCC\_A1                            BCC\_A2                            A2\_BCC  
HCP\_A3                            HCP\_ZN                            DIAMOND\_A4  
BCT\_A5                            TETRAGONAL\_A6                    RHOMBOHEDRAL\_A7  
CBCC\_A12                           CUB\_A13                           B32\_ALLI  
B3\_ZINCBLLENDE                   C14\_LAVES                           C15\_LAVES  
C16\_AL2CU                           C36\_LAVES                           D019\_AL1M3  
D513\_AL3NI2                           D82\_FEZN\_GAMMA                    L10\_ALTI  
AGZN\_ZETA                           AL5FE4                            ALCE\_AMORPHOUS  
ALCU\_ETA                           FEZN4                            FEZN\_DELTA  
FEZN\_ZETA   REJECTED  
LIQUID:L   RESTORED  
FCC\_A1   RESTORED  
HCP\_A3   RESTORED  
HCP\_ZN   RESTORED  
ELEMENTS   ....  
SPECIES   ....  
PHASES   ....  
PARAMETERS ...  
FUNCTIONS ....

List of references for assessed data

'A T Dinsdale, SGTE Data for Pure Elements, Calphad 15(1991)4 p 317-425; '

'A T Dinsdale, SGTE Data for Pure Elements, update 2001'

'S an Mey, Z Metallkde 84(1993)7 p 451-455; Al-Zn'

-OK-

Forcing automatic start values

Automatic start values will be set

No initial equilibrium, using default

Step will start from axis value   1000.000

...OK

Phase Region from   1000.000        for:

LIQUID  
Global test at   9.20000E+02   .... OK  
Global test at   8.20000E+02   .... OK  
Global check of adding phase at   7.88048E+02  
Calculated        24 equilibria

Phase Region from        788.048        for:

LIQUID  
FCC\_A1  
Global test at   7.26000E+02   .... OK  
Global test at   7.06000E+02   .... OK  
Global check of removing phase at   7.00299E+02  
Calculated        23 equilibria

Phase Region from        700.299        for:

FCC\_A1  
Global test at   6.28000E+02   .... OK  
Global test at   5.28000E+02   .. Backtracking to find phase change for FCC\_A1#2  
Global test at   6.18000E+02   .... OK  
Global test at   5.98000E+02   .... OK  
Global check of adding phase at   5.96831E+02  
Calculated        15 equilibria

Phase Region from        596.831        for:

FCC\_A1  
FCC\_A1#2  
Global check of adding phase at   5.50386E+02  
Calculated        7 equilibria

Phase Region from        550.386        for:

FCC\_A1  
FCC\_A1#2  
HCP\_ZN  
Calculated        2 equilibria

Phase Region from        550.386        for:

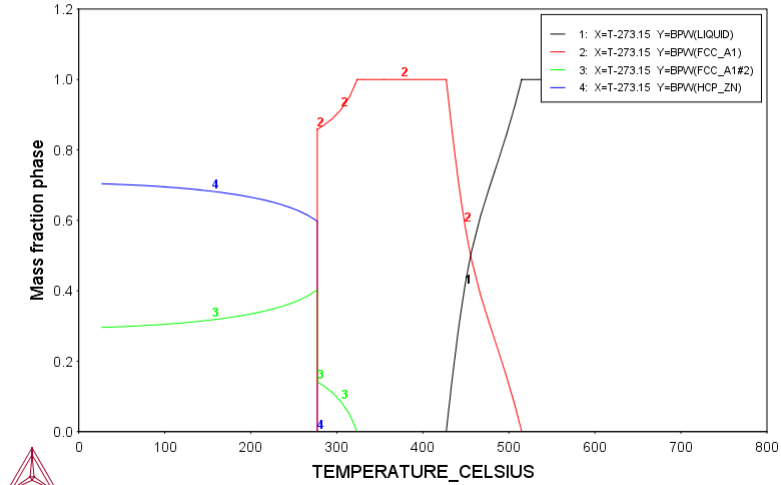
FCC\_A1#2  
HCP\_ZN  
Global test at   4.78000E+02   .... OK  
Global test at   3.78000E+02   .... OK  
Terminating at        300.000  
Calculated        29 equilibria  
\*\*\* Buffer saved on file:  
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex34\PFPU  
RVE.POLY3

POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

2016.05.16.14.16.24  
TCBIN: AL, ZN  
N=1, P=1E5, X(ZN)=0.5

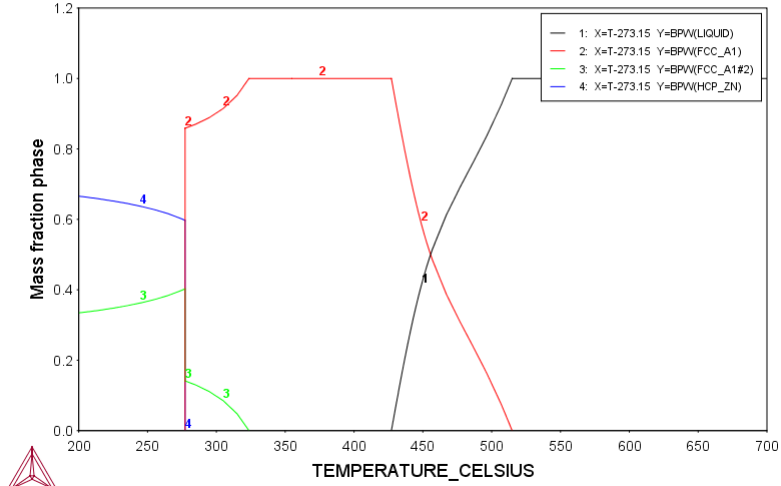
AL ZN



POST: s-s x n 200 700  
POST: set-title example 34d  
POST: plot

example 34d

2016.05.16.14.16.24  
TCBIN: AL, ZN  
N=1, P=1E5, X(ZN)=0.5



POST: set-inter

## tcex35

About Software (build 9533) running on WinNT 64-bit wordlength  
Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118  
License library version: 8.5.1.0017  
Linked: Mon May 16 09:31:44 2016

```
SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex35\tcex35.TCM"SYS: set-echo
SYS: @@
SYS: @@
SYS: @@ Example of use of the POTENTIAL module
SYS: @@
SYS: go pot
```

Simple potential phase diagram calculation module

Database: /POT/: SUBDEMO  
THERMODYNAMIC DATABASE module  
Current database: Substance Demo Database

```
VA /- DEFINED
Matrix element: /FE/: FE
First potential species: /S1O2/: C1O1
Second potential species: /O2/: O2
Temperature: /1000/: 1000
VA /- DEFINED
REINITIATING GES5 .....
FE C O
DEFINED
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....
```

List of references for assessed data

```
'C1<G> T.C.R.A.S. Class: 1 C1<G> C<G>'
'C1O1<G> JANAF THERMOCHEMICAL TABLES SGTE ** C1O1<G> CO<G> CARBON MONOXIDE
<GAS> STANDARD STATE : CODATA KEY VALUE. /CP FROM JANAF PUB. 9/65'
'C1O2<G> T.C.R.A.S. Class: 2 C1O2<G> CO2<G> CARBON DIOXIDE <GAS>'
'C2<G> T.C.R.A.S. Class: 2 C2<G> CARBON Diatomic Gas.'
'C2O1<G> T.C.R.A.S. Class: 5 C2O1<G> C2O<G>'
'C3<G> T.C.R.A.S. Class: 6 C3<G> CARBON <TRIATOMIC GAS>'
'C3O2<G> T.C.R.A.S. Class: 6 C3O2<G>'
'C4<G> T.C.R.A.S. Class: 7 C4<G>'
'C5<G> T.C.R.A.S. Class: 7 C5<G>'
'C5FE1O5<G> JANAF 1982 SGTE C5FE1O5<G> Fe(CO)5<G> IRON PENTACARBONYL <GAS>
ASSESSMENT DATED 3/78'
'C60<G> MHR-95 C60<G> Data processed from [94Kor/Sid] M.V. Korobov, L.N.
sidorov, J. Chem. Thermo, 26, 61-73 (1994). Recalculated from the
rotational data in [91McK] and vibration frequencies in [94Kor/Sid].
Note that a frequency with degeneracy 5 is missing from list in
[94Kor/Sid]; taken to be 419 cm-1, which gives very good, though not
exact, agreement with values quoted in [94Kor/Sid]. Note discrepancy
between calculated DrS(298) = -8943.5 J mol K-1 for the reaction 60C<g>
=C60<g>and that given by [94Kor/Sid] in their Table 5, -8950 J mol K
-1. Enthalpy of formation: DfH = 2588 kJ/mol from DsubH(298.15K) = 166
+/- 11 kJ mol-1 [94Kor/Sid]. Vapour pressure values reproduced very
well. [91McK] J.T. McKinnon, J. Phys. Chem. 95 8941(1993).'
```

```
'FE1<G> THERMODATA FE1<G> Fe<G> Data provided by T.C.R.A.S. October 1996
Modified by Thermodata - new assessment'
'FE1O1<G> TCRAS 5-F FEO IRON OXIDE 23/11/06 FE1O1<G> FeO<G>'
'FE1O2<G> T.C.R.A.S Class: 6 FE1O2<G> FeO2<G> Data provided by TCRAS.
October 1996. Error in version 1997. S298 corrected to 1bar 20080222
AAZ TCRAS2006 : dH, S'
'FE2<G> THERMODATA FE2<G> Fe2<G> Data provided by T.C.R.A.S. October 1996
Modified by Thermodata - new assessment. Typing error corrected 12/06'
'O2<G> TCRAS 21/06/90 O2<G> OXYGEN Gaseous Standard State.'
```

```
'O3<G> TCRAS 02/06/80 O3<G> OZONE Gaseous Standard State.'
```

```
'ClFE1O3 N.P.L. SGTE ** ClFE1O3 FeCO3 Siderite IRON<2> CARBONATE
DECOMPOSES BEFORE FUSION.'
```

```
'ClFE3 N.P.L. SGTE ** ClFE3 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  
\*\* FE101\_S  
FE\_S  
\*\* GRAPHITE

Phase region boundary 4 at: -9.383E-01 -5.007E+01  
\*\* FE101\_S  
FE\_S  
Calculated.. 151 equilibria  
Terminating at axis limit.

Phase region boundary 5 at: -9.383E-01 -5.007E+01  
\*\* FE101\_S  
GRAPHITE  
Calculated. 2 equilibria

Phase region boundary 6 at: -3.398E-01 -4.887E+01  
\*\* GAS  
\*\* FE101\_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  
FE101\_S  
Calculated. 7 equilibria

Phase region boundary 9 at: -3.272E+00 -4.059E+01  
\*\* GAS  
FE101\_S  
\*\* MAGNETITE

Phase region boundary 10 at: -3.272E+00 -4.059E+01  
FE101\_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  
\*\* FE101\_S  
FE\_S  
Calculated.. 81 equilibria  
Terminating at known equilibrium  
Terminating at axis limit.

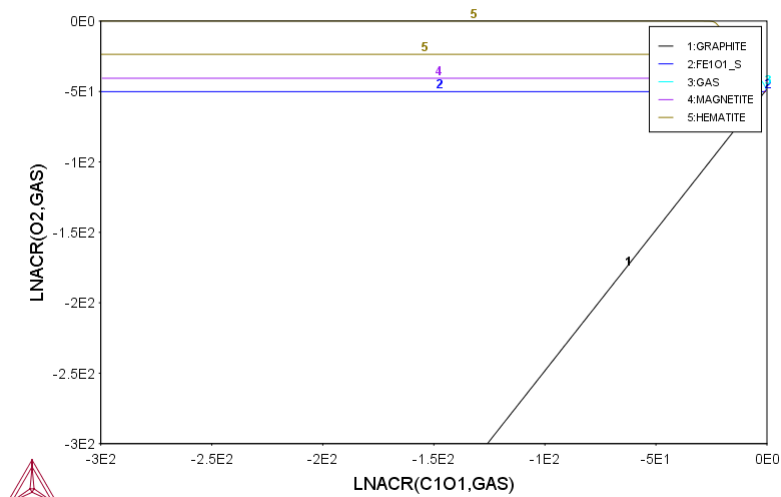
Phase region boundary 17 at: -1.409E+02 -5.007E+01  
\*\* FE101\_S  
FE\_S  
Calculated. 71 equilibria  
Terminating at known equilibrium  
\*\*\* BUFFER SAVED ON FILE:  
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex35\POT.  
POLY3  
CPU time for mapping 1 seconds

POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

FE C1O1 O2; Database: SUBDEMO

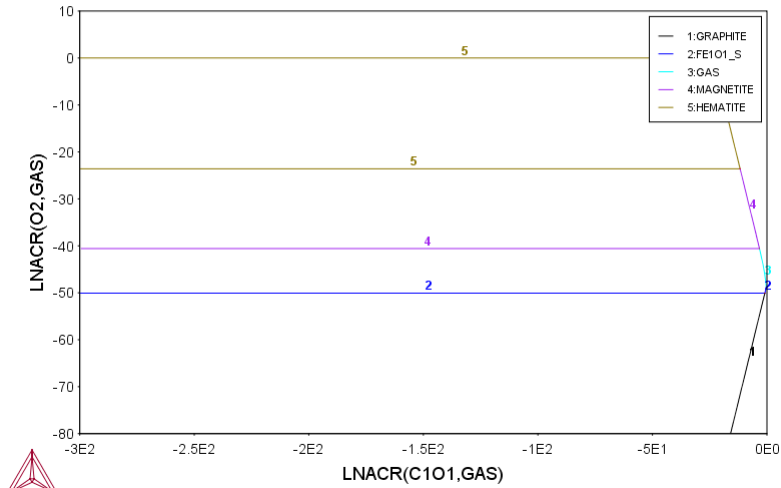
2016.05.16.14.17.57  
SUBDEMO: C, FE, O  
P=1E5, N=1, T=1000



POST: s-s y n -80 10  
POST: set-title example 35a  
POST:  
POST: pl

example 35a

2016.05.16.14.17.57  
SUBDEMO: C, FE, O  
P=1E5, N=1, T=1000



POST:  
POST: set-inter  
POST:

## tcex36a

```
SYS>AboutSYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tcex36a.TCM"SYS: set-echo
SYS: @@
SYS: @@ Assessment. The use of the PARROT module
SYS: @@
SYS: @@ This is the setup file for windows systems
SYS: @@
SYS: set_log tcex36a,,,,
SYS: @@ First the elements and phases must be entered in G-E-S module
SYS: GO G
... the command in full is GOTO_MODULE
GIBBS ENERGY SYSTEM version 5.2
GES: ENTER-ELEMENT A B
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
L12 FCC B2 BCC B2_VACANCY
HIGH SIGMA DICTRA FCC A1 REJECTED
GES: AMEND-ELEMENT-DATA A BCC 20 0 0 1
GES: AMEND-ELEMENT-DATA B BCC 50 0 0 1
GES: ENTER-PHASE LIQUID L 1 A B; N N
GES: ENTER-PHASE BCC,, 1 A B; N N
GES: ENTER-PHASE FCC,, 1 A B; N N
GES: ENTER-PHASE A2B,, 2 2 1 A; B; N N
CONSTITUENTS IN SUBLATTICE 1
CONSTITUENTS IN SUBLATTICE 2
GES: @@ There is a miscibility gap in the bcc, this must be stated here
GES: AMEND_PHASE BCC COMPOSITION_SETS 2 B
... the command in full is AMEND_PHASE_DESCRIPTION
GES: @@ We can also set the major constituent of the first composition set
GES: AMEND_PHASE BCC MAJOR 1 A
... the command in full is AMEND_PHASE_DESCRIPTION
GES:
GES: @@ The FCC phase is stable only for element B
GES: AMEND_PHASE FCC MAJOR 1 B
... the command in full is AMEND_PHASE_DESCRIPTION
GES: @@ the parameters can be entered in the PARROT module
GES: GO PAR
... the command in full is GOTO_MODULE

PARROT VERSION 5.3

Global minimization used as test only
PARROT: ENTER-PARAMETER G(BCC,A) 500 0; 2000 N
G(BCC,A;0)-G(BCC,A;0)
PARROT: ENTER-PARAMETER G(BCC,B) 500 0; 2000 N
G(BCC,B;0)-G(BCC,B;0)
PARROT: ENTER-PARAMETER G(LIQUID,A) 500 14000-10*T; 2000 N
G(LIQUID,A;0)-G(BCC,A;0)
PARROT: ENTER-PARAMETER G(LIQUID,B) 500 18000-12*T; 2000 N
G(LIQUID,B;0)-G(BCC,B;0)
PARROT: ENTER-PARAMETER G(FCC,B) 500 3300-3*T; 2000 N
G(FCC,B;0)-G(BCC,B;0)
PARROT: ENTER-PARAMETER G(FCC,A) 500 408; 2000 N
G(FCC,A;0)-G(BCC,A;0)
PARROT: ENTER-PARAMETER G(A2B) 500 V1+V2*T+V3*T*LOG(T); 2000 N
G(A2B,A;B;0)- 2 G(BCC,A;0)-G(BCC,B;0)
PARROT: ENTER-PARAMETER G(LIQUID,A,B;0) 500 V11+V12*T; 2000 N
G(LIQUID,A,B;0)
PARROT: ENTER-PARAMETER G(LIQUID,A,B;1) 500 V13+V14*T; 2000 N
G(LIQUID,A,B;1)
PARROT: ENTER-PARAMETER G(BCC,A,B;0) 500 V15+V16*T; 2000 N
G(BCC,A,B;0)
PARROT: ENTER-PARAMETER G(BCC,A,B;1) 500 V17+V18*T; 2000 N
G(BCC,A,B;1)
PARROT: ENTER-PARAMETER G(FCC,A,B;0) 500 V19+V20*T; 2000 N
G(FCC,A,B;0)
PARROT: ENTER-PARAMETER G(FCC,A,B;1) 500 V21+V22*T; 2000 N
G(FCC,A,B;1)
PARROT:
PARROT: @@ everything is saved on an unformatted work file by the create command
PARROT: CREATE tcex36
... the command in full is CREATE_NEW_STORE_FILE
PARROT:
PARROT:Hit RETURN to continue
PARROT:
PARROT: @@ the experimental data file is compiled to the work file.
PARROT: COMPILE tcex36 screen Y exp36
... the command in full is COMPILE_EXPERIMENTS
A new feature is that POP files may include graphics information using the
GRAPHICS_PLOT command. A file name for generating an ".exp" file must be given.
$
$ POP file for assessment example
$
$ Enter some constants used later.
ENTER_SYMBOL CONSTANT DX=0.02,P0=101325,DH=500,DT=10
$
$ Eutectic point at A rich side from ref #2.
$ T=1193 K, 40.8 w/o B in liquid, 13 w/o B in bcc.
$ In a binary system one must have four conditions if P is not fixed.
$ We obtain this by fixing the pressure and that three phases must be stable.
$ The amount of the fixed phases is irrelevant here
CREATE_NEW_EQUILIBRIUM 1,1
CHANGE_STATUS PHASE LIQUID,BCC,A2B=FIX 1
SET-CONDITION P=P0
EXPERIMENT T=1193:DT,W(LIQ,B)=.408:DX,W(BCC,B)=.13:DX
GRAPHICS 1 .408 1193 MS5
... the command in full is GRAPHICS_PLOT
GRAPHICS 1 .13 1193 DS5
... the command in full is GRAPHICS_PLOT
GRAPHICS 1 .555 1193 DS5
... the command in full is GRAPHICS_PLOT
LABEL AINV
... the command in full is LABEL_DATA
SET-ALT X(A2B,A)=.6666667
... the command in full is SET_ALTERNATE_CONDITION
SET_ALL_START 1193 Y
... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
$
```

```

$ Congrent melting temperature for A2B 1341 K.
$ We will include the enthalpy of transformation also and this
$ requires a function.
ENTER_SYMBOL FUNCTION HTR=HM(LIQUID)-HM(A2B);
$
$ Note how one specifies that this is a congruent transformation!
CREATE_NEW_EQUILIBRIUM 2,1
CHANGE_STATUS PHASE LIQ,A2B=FIX 1
SET-CONDITION P=P0,X(LIQ,B)-X(A2B,B)=0
EXPERIMENT T=1341:DT
EXPERIMENT HTR=3727:500
GRAPHICS 1 .555 1341 MS7
... the command in full is GRAPHICS_PLOT
LABEL AINV
... the command in full is LABEL_DATA
SET-ALT X(A)=.6666667
... the command in full is SET_ALTERNATE_CONDITION
SET_ALL_START 1341 Y
... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
$
$ Eutectic point at B rich side.
$ T=1049 K, 27 w/o A in liquid, 9.3 w/o A in bcc.
CREATE_NEW_EQUILIBRIUM 3,1
CHANGE_STATUS PHASE LIQ,BCC,A2B=FIX 1
SET-CONDITION P=P0
EXPERIMENT T=1049:DT,W(LIQ,A)=.27:DX,W(BCC,A)=.093:DX
SET-ALT X(A2B,A)=.6666667
... the command in full is SET_ALTERNATE_CONDITION
GRAPHICS 1 .907 1049 MS5
... the command in full is GRAPHICS_PLOT
GRAPHICS 1 .73 1049 DS5
... the command in full is GRAPHICS_PLOT
GRAPHICS 1 .555 1049 DS5
... the command in full is GRAPHICS_PLOT
LABEL AINV
... the command in full is LABEL_DATA
SET_ALL_START 1049 Y
... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
$
$ Peritectic point. T=1203 K, 19 w/o A in liquid, 6.9 w/o A in bcc,
$ 6.0 w/o A in fcc.
CREATE_NEW_EQUILIBRIUM 4,1
CHANGE_STATUS PHASE LIQ,BCC,FCC=FIX 1
SET-CONDITION P=P0
EXPERIMENT T=1203:DT,W(LIQ,A)=.19:DX,W(BCC,A)=.069:DX,W(FCC,A)=.06:DX
GRAPHICS 1 .81 1203 MS5
... the command in full is GRAPHICS_PLOT
GRAPHICS 1 .931 1203 DS5
... the command in full is GRAPHICS_PLOT
GRAPHICS 1 .94 1203 DS5
... the command in full is GRAPHICS_PLOT
LABEL AINV
... the command in full is LABEL_DATA
SET_ALL_START 1203 Y
... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
$
$ Eutectoid transformation of A2B -> BCC1 + BCC2, from ref #3
$ T=726, 3.7 at/o B in A, 11.4 at/o A in B
$ Note that miscibility gaps are indicated by using # after the phase
$ name and then give an integer.
CREATE_NEW_EQUILIBRIUM 5,1
CHANGE_STATUS PHASE BCC#1,BCC#2,A2B=FIX 1
SET-CONDITION P=P0
EXPERIMENT T=726:DT,X(BCC#1,B)=.037:DX,X(BCC#2,A)=.114:DX
SET-ALT X(A2B,A)=.6666667
... the command in full is SET_ALTERNATE_CONDITION
GRAPHICS 1 0.09 726 MS5
... the command in full is GRAPHICS_PLOT
GRAPHICS 1 0.95 726 DS5
... the command in full is GRAPHICS_PLOT
LABEL AINV
... the command in full is LABEL_DATA
SET_ALL_START 726 Y
... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
$
$ It is sometimes useful to decribe an invariant equilibria as
$ three tie-lines between each pair of phases at the same temperature.
$ In this case it helps to add a tie-line across the miscibility gap
$ at the invariant temperature.
CREATE_NEW_EQUILIBRIUM 6,1
CHANGE_STATUS PHASE BCC#1,BCC#2=FIX 1
SET-CONDITION P=P0 T=726
EXPERIMENT X(BCC#1,B)=.037:DX,X(BCC#2,A)=.114:DX
LABEL AINV
... the command in full is LABEL_DATA
SET_ALL_START Y
... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
$
$ From ref #4 the liquidus at the B rich end:
$ The table values are referenced inside the table_head using @<column>
TABLE HEAD 10
CREATE_NEW_EQUILIBRIUM 0010,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET-CONDITION T=1594,P=P0
EXPERIMENT W(LIQ,A)=0.02:DX
LABEL ALF
... the command in full is LABEL_DATA
GRAPHICS 1 .98 1594 MS5
... the command in full is GRAPHICS_PLOT
SET_ALL_START Y
... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0011,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET-CONDITION T=1548,P=P0
EXPERIMENT W(LIQ,A)=0.042:DX
LABEL ALF
... the command in full is LABEL_DATA
GRAPHICS 1 .958 1548 MS5
... the command in full is GRAPHICS_PLOT
SET_ALL_START Y

```



```

... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
CREATE_NEW EQUILIBRIUM 0012,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET-CONDITION T=1499,P=P0
EXPERIMENT W(LIQ,A)=0.065:DX
LABEL ALF
... the command in full is LABEL_DATA
GRAPHICS 1 .935 1499 MS5
... the command in full is GRAPHICS_PLOT
SET_ALL_START Y
... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
CREATE_NEW EQUILIBRIUM 0013,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET-CONDITION T=1438,P=P0
EXPERIMENT W(LIQ,A)=0.093:DX
LABEL ALF
... the command in full is LABEL_DATA
GRAPHICS 1 .907 1438 MS5
... the command in full is GRAPHICS_PLOT
SET_ALL_START Y
... the command in full is SET_ALL_START_VALUES
Automatic start values will be set

$
$ From ref #5 we have the following tie-lines
TABLE HEAD 20
CREATE_NEW EQUILIBRIUM 0020,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET-CONDITION T=1413,P=P0
EXPERIMENT W(LIQ,A)=.104:DX,W(FCC,A)=.038:DX
GRAPHICS 1 .896 1413 MS9
... the command in full is GRAPHICS_PLOT
GRAPHICS 1 .962 1413 DS9
... the command in full is GRAPHICS_PLOT
LABEL ATIE
... the command in full is LABEL_DATA
SET_ALL_START Y
... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
SET_START_VALUE Y(LIQ,A)=.104,Y(FCC,A)=.038
CREATE_NEW EQUILIBRIUM 0021,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET-CONDITION T=1337,P=P0
EXPERIMENT W(LIQ,A)=.136:DX,W(FCC,A)=.047:DX
GRAPHICS 1 .864 1337 MS9
... the command in full is GRAPHICS_PLOT
GRAPHICS 1 .953 1337 DS9
... the command in full is GRAPHICS_PLOT
LABEL ATIE
... the command in full is LABEL_DATA
SET_ALL_START Y
... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
SET_START_VALUE Y(LIQ,A)=.136,Y(FCC,A)=.047
CREATE_NEW EQUILIBRIUM 0022,1
CHANGE_STATUS PHASE LIQ,FCC=FIX 1
SET-CONDITION T=1213,P=P0
EXPERIMENT W(LIQ,A)=.187:DX,W(FCC,A)=.059:DX
GRAPHICS 1 .813 1213 MS9
... the command in full is GRAPHICS_PLOT
GRAPHICS 1 .941 1213 DS9
... the command in full is GRAPHICS_PLOT
LABEL ATIE
... the command in full is LABEL_DATA
SET_ALL_START Y
... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
SET_START_VALUE Y(LIQ,A)=.187,Y(FCC,A)=.059
CREATE_NEW EQUILIBRIUM 0023,1
CHANGE_STATUS PHASE LIQ,BCC=FIX 1
SET-CONDITION T=1100,P=P0
EXPERIMENT W(LIQ,A)=.245:DX,W(BCC,A)=.085:DX
GRAPHICS 1 .755 1100 MS9
... the command in full is GRAPHICS_PLOT
GRAPHICS 1 .915 1100 DS9
... the command in full is GRAPHICS_PLOT
LABEL ATIE
... the command in full is LABEL_DATA
SET_ALL_START Y
... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
SET_START_VALUE Y(LIQ,A)=.245,Y(BCC,A)=.085

$
$ Thermochemical data
$ Activities of B in liquid (reference state fcc) at 1573 K.
$ The command SET_REFERENCE_STATE is used for this as the default
$ reference state for B is BCC.
$
$ Note that we have set an uncertainty on the fraction (condition) also.
TABLE HEAD 100
CREATE_NEW EQUILIBRIUM 0100,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.90:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.94:DX
GRAPHICS 3 .90 .94 MS1
... the command in full is GRAPHICS_PLOT
LABEL AA
... the command in full is LABEL_DATA
CREATE_NEW EQUILIBRIUM 0101,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.80:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.84:DX
GRAPHICS 3 .80 .84 MS1
... the command in full is GRAPHICS_PLOT
LABEL AA
... the command in full is LABEL_DATA
CREATE_NEW EQUILIBRIUM 0102,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.70:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.74:DX

```

```

GRAPHICS 3 .70 .74 MS1
... the command in full is GRAPHICS_PLOT
LABEL AA
... the command in full is LABEL_DATA
CREATE_NEW_EQUILIBRIUM 0103,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.60:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.64:DX
GRAPHICS 3 .60 .64 MS1
... the command in full is GRAPHICS_PLOT
LABEL AA
... the command in full is LABEL_DATA
CREATE_NEW_EQUILIBRIUM 0104,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.50:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.54:DX
GRAPHICS 3 .50 .54 MS1
... the command in full is GRAPHICS_PLOT
LABEL AA
... the command in full is LABEL_DATA
CREATE_NEW_EQUILIBRIUM 0105,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.40:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.44:DX
GRAPHICS 3 .40 .44 MS1
... the command in full is GRAPHICS_PLOT
LABEL AA
... the command in full is LABEL_DATA
CREATE_NEW_EQUILIBRIUM 0106,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.30:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.34:DX
GRAPHICS 3 .30 .34 MS1
... the command in full is GRAPHICS_PLOT
LABEL AA
... the command in full is LABEL_DATA
CREATE_NEW_EQUILIBRIUM 0107,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.20:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.23:DX
GRAPHICS 3 .20 .23 MS1
... the command in full is GRAPHICS_PLOT
LABEL AA
... the command in full is LABEL_DATA
CREATE_NEW_EQUILIBRIUM 0108,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1573,P=P0,X(LIQ,B)=.10:DX
SET_REFERENCE_STATE B FCC,,,,
EXPERIMENT ACR(B)=.12:DX
GRAPHICS 3 .10 .12 MS1
... the command in full is GRAPHICS_PLOT
LABEL AA
... the command in full is LABEL_DATA

$
$ Enthalpy of mixing at 1773 K (reference state: liquid)
TABLE HEAD 110
CREATE_NEW_EQUILIBRIUM 0110,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1773,P=P0,X(LIQ,B)=.9
SET_REFERENCE_STATE A LIQ * 1E5
SET_REFERENCE_STATE B LIQ * 1E5
EXPERIMENT HMR(LIQ)=-1964:DH
GRAPHICS 2 .9 -1964 MS2
... the command in full is GRAPHICS_PLOT
LABEL AH
... the command in full is LABEL_DATA
SET_ALL_START Y
... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0111,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1773,P=P0,X(LIQ,B)=.8
SET_REFERENCE_STATE A LIQ * 1E5
SET_REFERENCE_STATE B LIQ * 1E5
EXPERIMENT HMR(LIQ)=-3500:DH
GRAPHICS 2 .8 -3500 MS2
... the command in full is GRAPHICS_PLOT
LABEL AH
... the command in full is LABEL_DATA
SET_ALL_START Y
... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0112,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1773,P=P0,X(LIQ,B)=.7
SET_REFERENCE_STATE A LIQ * 1E5
SET_REFERENCE_STATE B LIQ * 1E5
EXPERIMENT HMR(LIQ)=-4588:DH
GRAPHICS 2 .7 -4588 MS2
... the command in full is GRAPHICS_PLOT
LABEL AH
... the command in full is LABEL_DATA
SET_ALL_START Y
... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0113,1
CHANGE_STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1773,P=P0,X(LIQ,B)=.6
SET_REFERENCE_STATE A LIQ * 1E5
SET_REFERENCE_STATE B LIQ * 1E5
EXPERIMENT HMR(LIQ)=-5239:DH
GRAPHICS 2 .6 -5239 MS2
... the command in full is GRAPHICS_PLOT
LABEL AH
... the command in full is LABEL_DATA
SET_ALL_START Y
... the command in full is SET_ALL_START_VALUES
Automatic start values will be set
CREATE_NEW_EQUILIBRIUM 0114,1
CHANGE_STATUS PHASE LIQ=FIX 1

```

```

SET-CONDITION T=1773,P=P0,X(LIQ,B)=.5
SET-REFERENCE-STATE A LIQ * 1E5
SET-REFERENCE-STATE B LIQ * 1E5
EXPERIMENT HMR(LIQ)=-5454:DH
GRAPHICS 2 .5 -5454 MS2
... the command in full is GRAPHICS_PLOT
LABEL AH
... the command in full is LABEL_DATA
SET-ALL-START Y
... the command in full is SET-ALL-START-VALUES
Automatic start values will be set
CREATE-NEW-EQUILIBRIUM 0115,1
CHANGE-STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1773,P=P0,X(LIQ,B)=.4
SET-REFERENCE-STATE A LIQ * 1E5
SET-REFERENCE-STATE B LIQ * 1E5
EXPERIMENT HMR(LIQ)=-5233:DH
GRAPHICS 2 .4 -5233 MS2
... the command in full is GRAPHICS_PLOT
LABEL AH
... the command in full is LABEL_DATA
SET-ALL-START Y
... the command in full is SET-ALL-START-VALUES
Automatic start values will be set
CREATE-NEW-EQUILIBRIUM 0116,1
CHANGE-STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1773,P=P0,X(LIQ,B)=.3
SET-REFERENCE-STATE A LIQ * 1E5
SET-REFERENCE-STATE B LIQ * 1E5
EXPERIMENT HMR(LIQ)=-4575:DH
GRAPHICS 2 .3 -4575 MS2
... the command in full is GRAPHICS_PLOT
LABEL AH
... the command in full is LABEL_DATA
SET-ALL-START Y
... the command in full is SET-ALL-START-VALUES
Automatic start values will be set
CREATE-NEW-EQUILIBRIUM 0117,1
CHANGE-STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1773,P=P0,X(LIQ,B)=.2
SET-REFERENCE-STATE A LIQ * 1E5
SET-REFERENCE-STATE B LIQ * 1E5
EXPERIMENT HMR(LIQ)=-3481:DH
GRAPHICS 2 .2 -3481 MS2
... the command in full is GRAPHICS_PLOT
LABEL AH
... the command in full is LABEL_DATA
SET-ALL-START Y
... the command in full is SET-ALL-START-VALUES
Automatic start values will be set
CREATE-NEW-EQUILIBRIUM 0118,1
CHANGE-STATUS PHASE LIQ=FIX 1
SET-CONDITION T=1773,P=P0,X(LIQ,B)=.1
SET-REFERENCE-STATE A LIQ * 1E5
SET-REFERENCE-STATE B LIQ * 1E5
EXPERIMENT HMR(LIQ)=-1950:DH
GRAPHICS 2 .1 -1950 MS2
... the command in full is GRAPHICS_PLOT
LABEL AH
... the command in full is LABEL_DATA
SET-ALL-START Y
... the command in full is SET-ALL-START-VALUES
Automatic start values will be set

$
$ Heat of melting for the compound. T=1341. H(liq)-H(A2B)=3727 J/mol.
$ This datum has already been used.
$
$ Do not forget the following line!
SAVE-WORKSPACES
PARROT:
PARROT: @@
PARROT: @@ Next file shows how to guess rough start guess of the coefficients
PARROT: @@ and run the actual assessment. The values below are the final result.
PARROT: @@ S-O-V 1 20450,,,,,
PARROT: @@ S-O-V 2 -30.386,,,,,
PARROT: @@ S-O-V 3 0.131,,,,,
PARROT: @@ S-O-V 11 -21817,,,,,
PARROT: @@ S-O-V 12 15.34,,,,,
PARROT: @@ S-O-V 15 24212,,,,,
PARROT: @@ S-O-V 16 -8.328,,,,,
PARROT: @@ S-O-V 17 3105,,,,,
PARROT: @@ S-O-V 19 22030,,,,,
PARROT: @@ S-O-V 20 -6.981,,,,,
PARROT: @@ save the start guess on the work file
PARROT: s-o-v 1 0
... the command in full is SET-OPTIMIZING-VARIABLE
PARROT: s-o-v 2 0
... the command in full is SET-OPTIMIZING-VARIABLE
PARROT: s-o-v 11 0
... the command in full is SET-OPTIMIZING-VARIABLE
PARROT: s-o-v 12 0
... the command in full is SET-OPTIMIZING-VARIABLE
PARROT: s-o-v 15 0
... the command in full is SET-OPTIMIZING-VARIABLE
PARROT: s-o-v 16 0
... the command in full is SET-OPTIMIZING-VARIABLE
PARROT: s-o-v 17 0
... the command in full is SET-OPTIMIZING-VARIABLE
PARROT: s-o-v 19 0
... the command in full is SET-OPTIMIZING-VARIABLE
PARROT: s-o-v 20 0
... the command in full is SET-OPTIMIZING-VARIABLE
PARROT:
PARROT: save
... the command in full is SAVE-PARROT-WORKSPACES
PARROT: @@ Now executing tcex36b.TCM to continue the assessment example
PARROT: Hit RETURN to continue
PARROT: mac tcex36b.TCM
... the command in full is MACRO-FILE-OPEN
PARROT: s-s-f tcex36
... the command in full is SET-STORE-FILE
PARROT: @@ List parameters to be optimized, all zero initially
PARROT: l-a-v

```

```

... the command in full is LIST_ALL_VARIABLES
OUTPUT TO SCREEN OR FILE /SCREEN/:

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.  VALUE          START VALUE      SCALING FACTOR    REL.STAND.DEV
V1    0.00000000E+00  0.00000000E+00   1.00000000E+03   0.00000000E+00
V2    0.00000000E+00  0.00000000E+00   1.00000000E+03   0.00000000E+00
V11   0.00000000E+00  0.00000000E+00   1.00000000E+03   0.00000000E+00
V12   0.00000000E+00  0.00000000E+00   1.00000000E+03   0.00000000E+00
V15   0.00000000E+00  0.00000000E+00   1.00000000E+03   0.00000000E+00
V16   0.00000000E+00  0.00000000E+00   1.00000000E+03   0.00000000E+00
V17   0.00000000E+00  0.00000000E+00   1.00000000E+03   0.00000000E+00
V19   0.00000000E+00  0.00000000E+00   1.00000000E+03   0.00000000E+00
V20   0.00000000E+00  0.00000000E+00   1.00000000E+03   0.00000000E+00

NUMBER OF OPTIMIZING VARIABLES :    9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
PARROT: @@ Set alt mode to start
PARROT: s-alt Y
... the command in full is SET_ALTERNATE_MODE
PARROT: @@ Check if all equilibria can be calculated
PARROT: ed
... the command in full is EDIT_EXPERIMENTS
ED_EXP: read 1
... the command in full is READ_WORKSPACES
ED_EXP: c-a
... the command in full is COMPUTE_ALL_EQUILIBRIA
Eq Lab Iter Weight Temp Exp Fix phases or comments
 1 AINV *alt* 1.0 1193.0 LIQUID A2B BCC
 2 AINV *alt* 1.0 1341.0 LIQUID A2B
 3 AINV *alt* 1.0 1049.0 LIQUID A2B BCC
 4 AINV *alt* 1.0 1203.0 LIQUID BCC FCC
 5 AINV *alt* 1.0 726.0 A2B BCC BCC#2
 6 AINV *alt* 1.0 726.0 BCC BCC#2
Failed using alternate for FCC#1 setting weight to zero
10 ALF *alt* 1.0 1594.0 LIQUID FCC
Failed using alternate for FCC#1 setting weight to zero
11 ALF *alt* 1.0 1548.0 LIQUID FCC
Failed using alternate for FCC#1 setting weight to zero
12 ALF *alt* 1.0 1499.0 LIQUID FCC
Failed using alternate for FCC#1 setting weight to zero
13 ALF *alt* 1.0 1438.0 LIQUID FCC
20 ATIE *alt* 1.0 1413.0 LIQUID FCC
21 ATIE *alt* 1.0 1337.0 LIQUID FCC
22 ATIE *alt* 1.0 1213.0 LIQUID FCC
23 ATIE *alt* 1.0 1100.0 LIQUID BCC
100 AA 5 1. 1573.0 LIQUID
101 AA 4 1. 1573.0 LIQUID
102 AA 2 1. 1573.0 LIQUID
103 AA 3 1. 1573.0 LIQUID
104 AA 4 1. 1573.0 LIQUID
105 AA 6 1. 1573.0 LIQUID
106 AA 8 1. 1573.0 LIQUID
107 AA 9 1. 1573.0 LIQUID
108 AA 11 1. 1573.0 LIQUID
110 AH 8 1. 1773.0 LIQUID
111 AH 6 1. 1773.0 LIQUID
112 AH 5 1. 1773.0 LIQUID
113 AH 3 1. 1773.0 LIQUID
114 AH 2 1. 1773.0 LIQUID
115 AH 3 1. 1773.0 LIQUID
116 AH 5 1. 1773.0 LIQUID
117 AH 7 1. 1773.0 LIQUID
118 AH 8 1. 1773.0 LIQUID
Number of alternate equilibria 14
ED_EXP: @@ Equilibria with label ALF cannot use alt mode
ED_EXP: s-we 0 alf
... the command in full is SET_WEIGHT
Changed weight on 4 equilibria.
ED_EXP: c-a
... the command in full is COMPUTE_ALL_EQUILIBRIA
Eq Lab Iter Weight Temp Exp Fix phases or comments
118 AH 2 1. 1773.0 LIQUID
ED_EXP: save
... the command in full is SAVE_WORKSPACES
ED_EXP: @@ Save changes of weights before leaving editor
ED_EXP: ba
... the command in full is BACK
PARROT: @@ Optimize zero times as a check
PARROT: opt 0
... the command in full is OPTIMIZE_VARIABLES
Alternate calculation is on
Use 47 experiments, maximum is 2000
Use 1082 real workspace, maximum is 50000
PARROT: l-r C SCREEN
... the command in full is LIST_RESULT

=====
OUTPUT FROM P A R R O T. DATE 2016. 5.16 14:20: 7

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 0

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 0 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

== OPTIMIZING VARIABLES ==

```

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V2	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V11	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V12	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V15	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V16	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V17	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V19	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00
V20	0.00000000E+00	0.00000000E+00	1.00000000E+03	0.00000000E+00

NUMBER OF OPTIMIZING VARIABLES : 9  
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO  
THE SUM OF SQUARES HAS CHANGED FROM 0.00000000E+00 TO 1.22023362E+03  
DEGREES OF FREEDOM 38. REDUCED SUM OF SQUARES 3.21114110E+01

Number of alternate equilibria 10

SYMBOL	STATUS	VALUE/FUNCTION
1 R	80000000	8.3145100E+00
2 RTLNP	20000000	+R*T*LN(1E-05*P)

LIQUID  
EXCESS MODEL IS REDLICH-KISTER\_MUGGIANU  
CONSTITUENTS: A,B

G(LIQUID,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +14000-10\*T  
G(LIQUID,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +18000-12\*T  
L(LIQUID,A,B;0) = 500.00<T< 2000.00: +V11+V12\*T  
L(LIQUID,A,B;1) = 500.00<T< 2000.00: +V13+V14\*T

A2B  
2 SUBLATTICES, SITES 2: 1  
CONSTITUENTS: A : B

G(A2B,A;B;0) - 2 G(BCC,A;0) - G(BCC,B;0) =  
500.00<T< 2000.00: +V1+V2\*T+V3\*T\*LN(T)

BCC  
EXCESS MODEL IS REDLICH-KISTER\_MUGGIANU  
CONSTITUENTS: A,B

G(BCC,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +0.0  
G(BCC,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +0.0  
L(BCC,A,B;0) = 500.00<T< 2000.00: +V15+V16\*T  
L(BCC,A,B;1) = 500.00<T< 2000.00: +V17+V18\*T

FCC  
EXCESS MODEL IS REDLICH-KISTER\_MUGGIANU  
CONSTITUENTS: A,B

G(FCC,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +408  
G(FCC,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +3300-3\*T  
L(FCC,A,B;0) = 500.00<T< 2000.00: +V19+V20\*T  
L(FCC,A,B;1) = 500.00<T< 2000.00: +V21+V22\*T

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS

DX=2E-2, P0=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%

HTR=HM(LIQUID)-HM(A2B)

1 Alternate equilibrium calc					1.81	
2 Alternate equilibrium calc					0.39	
2 HTR=3727	1.5333E+04	5.00E+02	1.1606E+04	23.21	*	
3 Alternate equilibrium calc					1.32	
4 Alternate equilibrium calc					1.56	
5 Alternate equilibrium calc					4.14	
6 Alternate equilibrium calc					3.83	
20 Alternate equilibrium calc					0.87	
21 Alternate equilibrium calc					0.97	
22 Alternate equilibrium calc					1.14	
23 Alternate equilibrium calc					1.20	
100 ACR(B)=0.94	0.9382	2.89E-02	-1.8474E-03	-6.3948E-02		
101 ACR(B)=0.84	0.8339	2.89E-02	-6.0866E-03	-0.2107		
102 ACR(B)=0.74	0.7297	2.89E-02	-1.0326E-02	-0.3574		
103 ACR(B)=0.64	0.6254	2.89E-02	-1.4565E-02	-0.5042		
104 ACR(B)=0.54	0.5212	2.89E-02	-1.8804E-02	-0.6509		
105 ACR(B)=0.44	0.4170	2.89E-02	-2.3043E-02	-0.7976		
106 ACR(B)=0.34	0.3127	2.89E-02	-2.7282E-02	-0.9444		
107 ACR(B)=0.23	0.2085	2.89E-02	-2.1522E-02	-0.7450		
108 ACR(B)=0.12	0.1042	2.89E-02	-1.5761E-02	-0.5455		
110 HMR(LIQUID)=-1964	0.000	5.00E+02	1964.	3.928		
111 HMR(LIQUID)=-3500	0.000	5.00E+02	3500.	7.000	*	
112 HMR(LIQUID)=-4588	0.000	5.00E+02	4588.	9.176	*	
113 HMR(LIQUID)=-5239	-3.6380E-12	5.00E+02	5239.	10.48	*	
114 HMR(LIQUID)=-5454	1.8190E-12	5.00E+02	5454.	10.91	*	
115 HMR(LIQUID)=-5233	1.8190E-12	5.00E+02	5233.	10.47	*	
116 HMR(LIQUID)=-4575	-1.8190E-12	5.00E+02	4575.	9.150	*	
117 HMR(LIQUID)=-3481	0.000	5.00E+02	3481.	6.962	*	
118 HMR(LIQUID)=-1950	-1.8190E-12	5.00E+02	1950.	3.900		

PARROT:

PARROT:Hit RETURN to continue

PARROT: @@ Note only one error from alternate calculations. This error represents

PARROT: @@ the difference in chemical potentials of the phases.

PARROT: @@ Experiments with just one phase is calculated as normal.

PARROT: @@ Next command supresses listing of parameters.

PARROT: s-o-l 1 Y Y N n N

... the command in full is SET\_OUTPUT\_LEVELS

PARROT: l-r C SCREEN

... the command in full is LIST\_RESULT

\*\*\* SUCCESSFUL OPTIMIZATION. \*\*\*
NUMBER OF ITERATIONS: 0

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 0 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) \* 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR. VALUE START VALUE SCALING FACTOR REL.STAND.DEV
V1 0.00000000E+00 0.00000000E+00 1.00000000E+03 0.00000000E+00
V2 0.00000000E+00 0.00000000E+00 1.00000000E+03 0.00000000E+00
V11 0.00000000E+00 0.00000000E+00 1.00000000E+03 0.00000000E+00
V12 0.00000000E+00 0.00000000E+00 1.00000000E+03 0.00000000E+00
V15 0.00000000E+00 0.00000000E+00 1.00000000E+03 0.00000000E+00
V16 0.00000000E+00 0.00000000E+00 1.00000000E+03 0.00000000E+00
V17 0.00000000E+00 0.00000000E+00 1.00000000E+03 0.00000000E+00
V19 0.00000000E+00 0.00000000E+00 1.00000000E+03 0.00000000E+00
V20 0.00000000E+00 0.00000000E+00 1.00000000E+03 0.00000000E+00

NUMBER OF OPTIMIZING VARIABLES : 9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 0.00000000E+00 TO 1.22023362E+03
DEGREES OF FREEDOM 38. REDUCED SUM OF SQUARES 3.21114110E+01

Number of alternate equilibria 10

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS
DX=2E-2, P0=101325, DH=500, DT=10
DEFINED FUNCTIONS AND VARIABLES%
HTR=HM(LIQUID)-HM(A2B)
1 Alternate equilibrium calc 1.81
2 Alternate equilibrium calc 0.39
2 HTR=3727 1.5333E+04 5.00E+02 1.1606E+04 23.21 \*
3 Alternate equilibrium calc 1.32
4 Alternate equilibrium calc 1.56
5 Alternate equilibrium calc 4.14
6 Alternate equilibrium calc 3.83
20 Alternate equilibrium calc 0.87
21 Alternate equilibrium calc 0.97
22 Alternate equilibrium calc 1.14
23 Alternate equilibrium calc 1.20
100 ACR(B)=0.94 0.9382 2.89E-02 -1.8474E-03 -6.3948E-02
101 ACR(B)=0.84 0.8339 2.89E-02 -6.0866E-03 -0.2107
102 ACR(B)=0.74 0.7297 2.89E-02 -1.0326E-02 -0.3574
103 ACR(B)=0.64 0.6254 2.89E-02 -1.4565E-02 -0.5042
104 ACR(B)=0.54 0.5212 2.89E-02 -1.8804E-02 -0.6509
105 ACR(B)=0.44 0.4170 2.89E-02 -2.3043E-02 -0.7976
106 ACR(B)=0.34 0.3127 2.89E-02 -2.7282E-02 -0.9444
107 ACR(B)=0.23 0.2085 2.89E-02 -2.1522E-02 -0.7450
108 ACR(B)=0.12 0.1042 2.89E-02 -1.5761E-02 -0.5455
110 HMR(LIQUID)=-1964 0.000 5.00E+02 1964. 3.928
111 HMR(LIQUID)=-3500 0.000 5.00E+02 3500. 7.000 \*
112 HMR(LIQUID)=-4588 0.000 5.00E+02 4588. 9.176 \*
113 HMR(LIQUID)=-5239 -3.6380E-12 5.00E+02 5239. 10.48 \*
114 HMR(LIQUID)=-5454 1.8190E-12 5.00E+02 5454. 10.91 \*
115 HMR(LIQUID)=-5233 1.8190E-12 5.00E+02 5233. 10.47 \*
116 HMR(LIQUID)=-4575 -1.8190E-12 5.00E+02 4575. 9.150 \*
117 HMR(LIQUID)=-3481 0.000 5.00E+02 3481. 6.962 \*
118 HMR(LIQUID)=-1950 -1.8190E-12 5.00E+02 1950. 3.900

PARROT:

PARROT: @@ Now optimize

PARROT: opt 30

... the command in full is OPTIMIZE\_VARIABLES
Alternate calculation is on
Use 47 experiments, maximum is 2000
Use 1082 real workspace, maximum is 50000
The following output is provided by subroutine VA05A

AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 1.22023362E+03
1 0.0000E+00 2 0.0000E+00 3 0.0000E+00 4 0.0000E+00 5 0.0000E+00
6 0.0000E+00 7 0.0000E+00 8 0.0000E+00 9 0.0000E+00
AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 1.22023056E+03
1 1.0000E-04 2 0.0000E+00 3 0.0000E+00 4 0.0000E+00 5 0.0000E+00
6 0.0000E+00 7 0.0000E+00 8 0.0000E+00 9 0.0000E+00
AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 1.22026107E+03
1 1.0000E-04 2 1.0000E-04 3 0.0000E+00 4 0.0000E+00 5 0.0000E+00
6 0.0000E+00 7 0.0000E+00 8 0.0000E+00 9 0.0000E+00
AT THE 3 RD ITERATION WE HAVE THE SUM OF SQUARES 1.22023821E+03
1 1.0000E-04 2 0.0000E+00 3 1.0000E-04 4 0.0000E+00 5 0.0000E+00
6 0.0000E+00 7 0.0000E+00 8 0.0000E+00 9 0.0000E+00
AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 1.21985896E+03
1 1.0000E-04 2 0.0000E+00 3 0.0000E+00 4 1.0000E-04 5 0.0000E+00
6 0.0000E+00 7 0.0000E+00 8 0.0000E+00 9 0.0000E+00
AT THE 5 TH ITERATION WE HAVE THE SUM OF SQUARES 1.21985855E+03
1 1.0000E-04 2 0.0000E+00 3 0.0000E+00 4 1.0000E-04 5 1.0000E-04
6 0.0000E+00 7 0.0000E+00 8 0.0000E+00 9 0.0000E+00

```

      AT THE      6 TH ITERATION WE HAVE THE SUM OF SQUARES      1.21952877E+03
1  1.0000E-04    2  0.0000E+00    3  0.0000E+00    4  1.0000E-04    5  1.0000E-04
6  1.0000E-04    7  0.0000E+00    8  0.0000E+00    9  0.0000E+00

      AT THE      7 TH ITERATION WE HAVE THE SUM OF SQUARES      1.21952862E+03
1  1.0000E-04    2  0.0000E+00    3  0.0000E+00    4  1.0000E-04    5  1.0000E-04
6  1.0000E-04    7  1.0000E-04    8  0.0000E+00    9  0.0000E+00

      AT THE      8 TH ITERATION WE HAVE THE SUM OF SQUARES      1.21952856E+03
1  1.0000E-04    2  0.0000E+00    3  0.0000E+00    4  1.0000E-04    5  1.0000E-04
6  1.0000E-04    7  1.0000E-04    8  1.0000E-04    9  0.0000E+00

      AT THE      9 TH ITERATION WE HAVE THE SUM OF SQUARES      1.21945175E+03
1  1.0000E-04    2  0.0000E+00    3  0.0000E+00    4  1.0000E-04    5  1.0000E-04
6  1.0000E-04    7  1.0000E-04    8  1.0000E-04    9  1.0000E-04

      AT THE     10 TH ITERATION WE HAVE THE SUM OF SQUARES      1.21347918E+03
1  1.1575E-04    2 -1.5562E-04    3 -3.9485E-05    4  1.9219E-03    5  1.0209E-04
6  1.7933E-03    7  1.0073E-04    8  1.0031E-04    9  4.9349E-04

      AT THE     11 TH ITERATION WE HAVE THE SUM OF SQUARES      1.20857820E+03
1  5.7604E-04    2 -2.8000E-04    3 -5.5554E-04    4  2.9761E-04    5  1.0310E-03
6  3.2119E-03    7  1.5940E-04    8  5.6559E-04    9  8.6813E-04

      AT THE     12 TH ITERATION WE HAVE THE SUM OF SQUARES      1.20419111E+03
1  1.7517E-03    2 -4.0933E-04    3 -1.8427E-03    4  1.7341E-03    5  1.9072E-03
6  4.5182E-03    7  3.6464E-04    8 -3.6442E-03    9  1.2034E-03

      AT THE     13 TH ITERATION WE HAVE THE SUM OF SQUARES      1.20018978E+03
1  4.9647E-03    2 -5.3990E-04    3 -5.3422E-03    4  4.2170E-04    5  1.3348E-03
6  5.8647E-03    7  1.0916E-03    8 -1.0101E-02    9  1.5910E-03

      AT THE     14 TH ITERATION WE HAVE THE SUM OF SQUARES      1.19656103E+03
1  8.7053E-03    2 -6.5937E-04    3 -9.4048E-03    4  1.6713E-03    5  2.0976E-03
6  6.9625E-03    7  1.8270E-03    8 -2.5618E-02    9  1.9085E-03

      AT THE     15 TH ITERATION WE HAVE THE SUM OF SQUARES      1.19290093E+03
1  1.6702E-02    2 -7.8966E-04    3 -1.8062E-02    4  5.3932E-04    5  2.8050E-03
6  8.1461E-03    7  3.5323E-03    8 -5.6536E-02    9  2.2985E-03

      AT THE     16 TH ITERATION WE HAVE THE SUM OF SQUARES      1.18895829E+03
1  2.9858E-02    2 -9.1157E-04    3 -3.2288E-02    4  1.6316E-03    5  6.0830E-03
6  9.0741E-03    7  6.1592E-03    8 -1.1985E-01    9  2.6324E-03

      AT THE     17 TH ITERATION WE HAVE THE SUM OF SQUARES      1.18371835E+03
1  5.7117E-02    2 -1.0621E-03    3 -6.1739E-02    4  6.6639E-04    5  1.1597E-02
6  1.0112E-02    7  1.1749E-02    8 -2.4612E-01    9  3.0842E-03

      AT THE     18 TH ITERATION WE HAVE THE SUM OF SQUARES      1.17576307E+03
1  1.0981E-01    2 -1.2302E-03    3 -1.1865E-01    4  1.6444E-03    5  2.3336E-02
6  1.0904E-02    7  2.2419E-02    8 -4.9950E-01    9  3.5580E-03

      AT THE     19 TH ITERATION WE HAVE THE SUM OF SQUARES      1.17580508E+03
1  1.0990E-01    2 -1.2331E-03    3 -1.1866E-01    4  1.6767E-03    5  2.3332E-02
6  1.0908E-02    7  2.2420E-02    8 -4.9948E-01    9  3.5631E-03

      AT THE     20 TH ITERATION WE HAVE THE SUM OF SQUARES      1.17576898E+03
1  1.0981E-01    2 -1.1307E-03    3 -1.1865E-01    4  1.6454E-03    5  2.3336E-02
6  1.0913E-02    7  2.2419E-02    8 -4.9950E-01    9  3.5581E-03

      AT THE     21 TH ITERATION WE HAVE THE SUM OF SQUARES      1.17573278E+03
1  1.0983E-01    2 -1.2301E-03    3 -1.1856E-01    4  1.6164E-03    5  2.3339E-02
6  1.0901E-02    7  2.2419E-02    8 -4.9952E-01    9  3.5536E-03

      AT THE     22 TH ITERATION WE HAVE THE SUM OF SQUARES      1.15839209E+03
1  2.4518E-01    2 -1.5171E-03    3 -2.6482E-01    4  8.9861E-04    5  8.1375E-02
6  1.1834E-02    7  4.7658E-02    8 -9.8754E-01    9  4.3315E-03

      AT THE     23 TH ITERATION WE HAVE THE SUM OF SQUARES      1.15852291E+03
1  2.4519E-01    2 -1.5109E-03    3 -2.6483E-01    4  8.8627E-04    5  8.1444E-02
6  1.1766E-02    7  4.7657E-02    8 -9.8753E-01    9  4.3220E-03

      AT THE     24 TH ITERATION WE HAVE THE SUM OF SQUARES      1.12429808E+03
1  5.3085E-01    2 -1.9804E-03    3 -5.7319E-01    4  1.9224E-03    5  3.5639E-01
6  1.2271E-02    7  9.3910E-02    8 -1.9219E+00    9  5.3987E-03

      AT THE     25 TH ITERATION WE HAVE THE SUM OF SQUARES      1.12430368E+03
1  5.3084E-01    2 -1.9806E-03    3 -5.7319E-01    4  1.9278E-03    5  3.5639E-01
6  1.2272E-02    7  9.4010E-02    8 -1.9219E+00    9  5.3997E-03

      AT THE     26 TH ITERATION WE HAVE THE SUM OF SQUARES      1.05801747E+03
1  1.1108E+00    2 -2.8497E-03    3 -1.1990E+00    4  1.6568E-03    5  1.0413E+00
6  1.2349E-02    7  1.7987E-01    8 -3.7400E+00    9  7.2585E-03

      AT THE     27 TH ITERATION WE HAVE THE SUM OF SQUARES      1.05799597E+03
1  1.1108E+00    2 -2.8479E-03    3 -1.1990E+00    4  1.6562E-03    5  1.0413E+00
6  1.2329E-02    7  1.7987E-01    8 -3.7401E+00    9  7.3562E-03

      AT THE     28 TH ITERATION WE HAVE THE SUM OF SQUARES      9.32316420E+02
1  2.2754E+00    2 -4.5180E-03    3 -2.4557E+00    4  3.1330E-03    5  2.5155E+00
6  1.1608E-02    7  3.4709E-01    8 -7.3322E+00    9  1.0723E-02

      AT THE     29 TH ITERATION WE HAVE THE SUM OF SQUARES      9.32175579E+02
1  2.2754E+00    2 -4.5239E-03    3 -2.4557E+00    4  3.0908E-03    5  2.5156E+00
6  1.1674E-02    7  3.4709E-01    8 -7.3322E+00    9  1.0740E-02

      AT THE     30 TH ITERATION WE HAVE THE SUM OF SQUARES      9.32266522E+02
1  2.2754E+00    2 -4.5260E-03    3 -2.4557E+00    4  3.1696E-03    5  2.5156E+00
6  1.1696E-02    7  3.4708E-01    8 -7.3322E+00    9  1.0745E-02

*** ERROR RETURN FROM VA05A BECAUSE THERE HAVE BEEN      30 CALLS OF CALFUN

      THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED      30 iterations
1  2.2754E+00    2 -4.5239E-03    3 -2.4557E+00    4  3.0908E-03    5  2.5156E+00
6  1.1674E-02    7  3.4709E-01    8 -7.3322E+00    9  1.0740E-02

1  2.7586E-01    2  2.7586E-01    3 -2.3479E-02    4 -2.9092E-01    5 -1.4825E-01
6 -2.4894E-01    7  2.0604E+01    8  1.1427E-01    9  1.1427E-01   10 -2.1551E-01
11 -1.4793E-01   12  6.1401E-02   13 -4.3625E-02   14 -7.7890E-01   15 -8.0449E-02
16  4.8856E-01   17  4.8856E-01   18 -7.3181E-01   19  1.4636E+00   20 -7.3181E-01
21  1.4636E+00   22 -4.1620E-01   23 -1.1022E-02   24 -5.4162E-01   25 -2.8760E-02
26 -7.6572E-01   27 -7.3156E-02   28 -1.2544E-01   29 -1.0373E-01   30 -4.2177E-03
31  2.5902E-03   32  6.6372E-02   33  1.4719E-01   34  2.0341E-01   35  1.9322E-01
36  7.6393E-02   37  1.5206E-01   38  3.2168E-02   39  3.4860E+00   40  6.2142E+00
41  8.1446E+00   42  9.2993E+00   43  9.6801E+00   44  9.2873E+00   45  8.1186E+00

```

46 6.1762E+00 47 3.4580E+00

THE SUM OF SQUARES IS 9.32175579E+02

PARROT: cont 30

... the command in full is CONTINUE\_OPTIMIZATION

Alternate calculation is on

Use 47 experiments, maximum is 2000

Use 1082 real workspace, maximum is 50000

The following output is provided by subroutine VA05A

Optimization continuing with same Jacobian

AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 6.42378436E+02  
1 5.3285E+00 2 -8.7738E-03 3 -5.7409E+00 4 4.7675E-03 5 5.1386E+00  
6 9.8927E-03 7 8.7846E-01 8 -1.4032E+01 9 1.6957E-02

AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 3.93287140E+02  
1 8.5798E+00 2 -1.3317E-02 3 -9.2391E+00 4 7.4937E-03 5 8.0040E+00  
6 7.9956E-03 7 1.4404E+00 8 -2.1386E+01 9 2.3783E-02

AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 2.09581259E+02  
1 1.1739E+01 2 -1.7636E-02 3 -1.2638E+01 4 9.3818E-03 5 1.0889E+01  
6 5.4398E-03 7 1.9808E+00 8 -2.8820E+01 9 3.0390E-02

AT THE 3 RD ITERATION WE HAVE THE SUM OF SQUARES 1.80919629E+01  
1 1.7814E+01 2 -2.5900E-02 3 -1.9174E+01 4 1.3734E-02 5 1.6703E+01  
6 -6.1201E-06 7 3.0058E+00 8 -4.3892E+01 9 4.3587E-02

AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 9.80059382E-01  
1 2.0269E+01 2 -2.9190E-02 3 -2.1813E+01 4 1.5556E-02 5 1.9856E+01  
6 -3.2628E-03 7 3.3757E+00 8 -5.2038E+01 9 5.0439E-02

THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 4 iterations  
1 2.0269E+01 2 -2.9190E-02 3 -2.1813E+01 4 1.5556E-02 5 1.9856E+01  
6 -3.2628E-03 7 3.3757E+00 8 -5.2038E+01 9 5.0439E-02

1 -1.6298E-03 2 -1.6298E-03 3 1.8275E-04 4 1.5454E-01 5 1.3483E-01  
6 -1.3372E-01 7 5.3414E-03 8 -1.9207E-03 9 -1.9207E-03 10 5.9902E-02  
11 -5.3043E-03 12 1.0919E-01 13 -3.1490E-03 14 -3.7871E-01 15 -1.5089E-02  
16 2.6188E-02 17 2.6188E-02 18 -1.0466E-01 19 6.6482E-02 20 -1.0466E-01  
21 6.6482E-02 22 4.7595E-01 23 4.3175E-03 24 1.7990E-01 25 -3.8166E-04  
26 -3.4079E-01 27 -1.0881E-02 28 7.4581E-02 29 -2.7851E-03 30 2.1227E-03  
31 2.5569E-02 32 1.1253E-01 33 2.1861E-01 34 2.9732E-01 35 3.0190E-01  
36 1.8750E-01 37 2.4843E-01 38 9.3003E-02 39 1.7059E-03 40 1.9922E-02  
41 1.4647E-02 42 7.8823E-03 43 1.6274E-03 44 -4.1177E-03 45 -1.1353E-02  
46 -1.8078E-02 47 -2.6294E-02

THE SUM OF SQUARES IS 9.80059382E-01

PARROT: l-r C SCREEN

... the command in full is LIST\_RESULT

=====

OUTPUT FROM P A R R O T. DATE 2016. 5.16 14:20: 8

\*\*\* OPTIMIZATION ERROR. TOO MANY ITERATIONS \*\*\*  
NUMBER OF ITERATIONS: 5

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N  
MINIMUM SAVE ON FILE: Y  
ERROR FOR INEQUALITIES = 1.00000000E+00  
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04  
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)  
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04  
ACC = (INITIAL SUM OF SQUARES) \* 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.02691580E+04	0.00000000E+00	1.00000000E+03	1.60588759E+00
V2	-2.91902505E+01	0.00000000E+00	1.00000000E+03	1.00991507E-02
V11	-2.18127452E+04	0.00000000E+00	1.00000000E+03	8.65821611E-01
V12	1.5559572E+01	0.00000000E+00	1.00000000E+03	2.63407916E-03
V15	1.98562648E+04	0.00000000E+00	1.00000000E+03	1.43531758E+01
V16	-3.26280484E+00	0.00000000E+00	1.00000000E+03	1.71198002E-02
V17	3.37569790E+03	0.00000000E+00	1.00000000E+03	4.53503022E+00
V19	-5.20381430E+04	0.00000000E+00	1.00000000E+03	3.15147730E+01
V20	5.04393965E+01	0.00000000E+00	1.00000000E+03	2.47939786E-02

NUMBER OF OPTIMIZING VARIABLES : 9  
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO  
THE SUM OF SQUARES HAS CHANGED FROM 1.22023362E+03 TO 9.80059382E-01  
DEGREES OF FREEDOM 38. REDUCED SUM OF SQUARES 2.57910364E-02

Number of alternate equilibria 10

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS

DX=2E-2, P0=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%

HTR=HM(LIQUID)-HM(A2B)

1	Alternate equilibrium calc				0.15
2	Alternate equilibrium calc				0.19
2	HTR=3727	3730.	5.00E+02	2.671	5.3414E-03
3	Alternate equilibrium calc				0.06
4	Alternate equilibrium calc				0.39
5	Alternate equilibrium calc				0.13
6	Alternate equilibrium calc				0.12
20	Alternate equilibrium calc				0.48
21	Alternate equilibrium calc				0.18
22	Alternate equilibrium calc				0.34
23	Alternate equilibrium calc				0.07
100	ACR(B)=0.94	0.9401	2.84E-02	6.0229E-05	2.1227E-03



101	ACR(B)=0.84	0.8407	2.80E-02	7.1694E-04	2.5569E-02
102	ACR(B)=0.74	0.7431	2.79E-02	3.1371E-03	0.1125
103	ACR(B)=0.64	0.6461	2.79E-02	6.0969E-03	0.2186
104	ACR(B)=0.54	0.5483	2.81E-02	8.3480E-03	0.2973
105	ACR(B)=0.44	0.4486	2.85E-02	8.5911E-03	0.3019
106	ACR(B)=0.34	0.3454	2.90E-02	5.4464E-03	0.1875
107	ACR(B)=0.23	0.2374	2.99E-02	7.4229E-03	0.2484
108	ACR(B)=0.12	0.1229	3.10E-02	2.8826E-03	9.3003E-02
110	HMR(LIQUID)=-1964	-1963.	5.00E+02	0.8529	1.7059E-03
111	HMR(LIQUID)=-3500	-3490.	5.00E+02	9.961	1.9922E-02
112	HMR(LIQUID)=-4588	-4581.	5.00E+02	7.324	1.4647E-02
113	HMR(LIQUID)=-5239	-5235.	5.00E+02	3.941	7.8823E-03
114	HMR(LIQUID)=-5454	-5453.	5.00E+02	0.8137	1.6274E-03
115	HMR(LIQUID)=-5233	-5235.	5.00E+02	-2.059	-4.1177E-03
116	HMR(LIQUID)=-4575	-4581.	5.00E+02	-5.676	-1.1353E-02
117	HMR(LIQUID)=-3481	-3490.	5.00E+02	-9.039	-1.8078E-02
118	HMR(LIQUID)=-1950	-1963.	5.00E+02	-13.15	-2.6294E-02

**PARROT:**  
**PARROT:Hit RETURN to continue**  
**PARROT:** @@ The liquid data fitted reasonable, fix its parameters to simplify  
**PARROT:** l-p-d liq  
 ... the command in full is LIST\_PHASE\_DATA

LIQUID  
 EXCESS MODEL IS REDLICH-KISTER\_MUGGIANU  
 CONSTITUENTS: A,B

G(LIQUID,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +14000-10\*T  
 G(LIQUID,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +18000-12\*T  
 L(LIQUID,A,B;0) = 500.00<T< 2000.00: +V11+V12\*T  
 L(LIQUID,A,B;1) = 500.00<T< 2000.00: +V13+V14\*T

**PARROT:** s-f-v 11-14  
 ... the command in full is SET\_FIX\_VARIABLE  
**PARROT:** @@ Rescale the start values of the parameters to current values  
**PARROT:** resc  
 ... the command in full is RESCALE\_VARIABLES  
**PARROT:** l-a-v  
 ... the command in full is LIST\_ALL\_VARIABLES  
**OUTPUT TO SCREEN OR FILE /SCREEN/:**

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.02691580E+04	2.02691580E+04	2.02691580E+04	0.00000000E+00
V2	-2.91902505E+01	-2.91902505E+01	-2.91902505E+01	0.00000000E+00
V11	-2.18127452E+04			
V12	1.55559572E+01			
V15	1.98562648E+04	1.98562648E+04	1.98562648E+04	0.00000000E+00
V16	-3.26280484E+00	-3.26280484E+00	-3.26280484E+00	0.00000000E+00
V17	3.37569790E+03	3.37569790E+03	3.37569790E+03	0.00000000E+00
V19	-5.20381430E+04	-5.20381430E+04	-5.20381430E+04	0.00000000E+00
V20	5.04393965E+01	5.04393965E+01	5.04393965E+01	0.00000000E+00

NUMBER OF OPTIMIZING VARIABLES : 7  
 ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO

**PARROT:Hit RETURN to continue**  
**PARROT:** mac tcex36cpd  
 ... the command in full is MACRO\_FILE\_OPEN  
**PARROT:** set-echo  
 NO SUCH COMMAND, USE HELP  
**PARROT:** @@ Calculate the phase diagram  
**PARROT:** @@ This TCM should be run in PARROT  
**PARROT:** go p-3  
 ... the command in full is GOTO\_MODULE  
**POLY\_3:**  
**POLY\_3:** @@ In PARROT, the global minimization is turned off automatically.  
**POLY\_3:** @@ Back in POLY-3, one needs to turn it on manually, but a warning  
**POLY\_3:** @@ message will be given.

**POLY\_3:** advanced-option global yes,,  
 ... the command in full is ADVANCED\_OPTIONS  
 Settings for global minimization:  
 \*\*\* WARNING \*\*\* Global equilibrium calculation may create new composition sets  
 and this may corrupt your PARROT work file (.PAR file).  
 Do not go back to PARROT but exit from POLY after your POLY calculations.

**POLY\_3:**  
**POLY\_3:** def-com,,,

... the command in full is DEFINE\_COMPONENTS

**POLY\_3:** s-a-v 1 w(b) 0 1,,,

... the command in full is SET\_AXIS\_VARIABLE  
 The condition W(B)=.1234 created

**POLY\_3:** s-a-v 2 t 300 1700,,,

... the command in full is SET\_AXIS\_VARIABLE  
 The condition T=942.2 created

**POLY\_3:** s-c t=500

... the command in full is SET\_CONDITION

**POLY\_3:** l-c

... the command in full is LIST\_CONDITIONS  
 W(B)=0.1234, P=1E5, N=1, T=500

DEGREES OF FREEDOM 0

**POLY\_3:** c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Using global minimization procedure

Calculated 412 grid points in 0 s

Found the set of lowest grid points in 0 s

Calculated POLY solution 0 s, total time 0 s

**POLY\_3:** save tcex36 y

... the command in full is SAVE\_WORKSPACES

**POLY\_3:** map

Version 8 mapping is selected

Generating start equilibrium 1

Generating start equilibrium 2

Generating start equilibrium 3

Generating start equilibrium 4

Generating start equilibrium 5

Generating start equilibrium 6

Generating start equilibrium 7

Generating start equilibrium 8

Generating start equilibrium 9

Generating start equilibrium 10  
Generating start equilibrium 11  
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1  
Generating start point 2  
Generating start point 3  
Generating start point 4  
Generating start point 5  
Generating start point 6  
Generating start point 7  
Generating start point 8  
Generating start point 9  
Generating start point 10

Working hard

Generating start point 11  
Generating start point 12  
Generating start point 13  
Generating start point 14  
Generating start point 15  
Generating start point 16  
Generating start point 17  
Generating start point 18  
Generating start point 19  
Generating start point 20

Working hard

Generating start point 21  
Generating start point 22  
Generating start point 23  
Generating start point 24  
Generating start point 25  
Generating start point 26  
Generating start point 27  
Generating start point 28

Phase region boundary 1 at: 8.907E-02 3.100E+02

BCC

\*\* FCC

Calculated.. 2 equilibria

Terminating at axis limit.

Phase region boundary 2 at: 8.956E-02 3.000E+02

BCC

\*\* FCC

Calculated. 29 equilibria

Phase region boundary 3 at: 1.213E-01 1.253E+03

\*\* LIQUID

BCC

\*\* FCC

Phase region boundary 4 at: 2.038E-01 1.253E+03

\*\* LIQUID

BCC

Calculated 26 equilibria

Phase region boundary 5 at: 2.413E-01 1.253E+03

\*\* LIQUID

FCC

Calculated. 6 equilibria

Phase region boundary 6 at: 3.546E-01 1.219E+03

\*\* LIQUID

\*\* A2B

FCC

Phase region boundary 7 at: 4.342E-01 1.219E+03

\*\* A2B

FCC

Calculated. 24 equilibria

Phase region boundary 8 at: 6.572E-01 1.191E+03

\*\* LIQUID

\*\* A2B

FCC

Phase region boundary 9 at: 7.154E-01 1.191E+03

\*\* LIQUID

FCC

Calculated 43 equilibria

Phase region boundary 10 at: 6.257E-01 1.191E+03

\*\* LIQUID

A2B

Calculated. 23 equilibria

Terminating at known equilibrium

Phase region boundary 11 at: 8.907E-02 3.100E+02

BCC

\*\* FCC

Calculated. 28 equilibria

Terminating at known equilibrium

Phase region boundary 12 at: 8.907E-02 3.100E+02

BCC

\*\* FCC

Calculated.. 2 equilibria

Terminating at known equilibrium

Terminating at axis limit.

Phase region boundary 13 at: 8.907E-02 3.100E+02

BCC

\*\* FCC

Calculated. 28 equilibria

Terminating at known equilibrium

Phase region boundary 14 at: 4.559E-01 1.196E+03

\*\* A2B

FCC

Calculated. 3 equilibria

Terminating at known equilibrium

Phase region boundary 15 at: 4.559E-01 1.196E+03  
 \*\* A2B  
 FCC  
 Calculated. 21 equilibria  
 Terminating at known equilibrium

Phase region boundary 16 at: 6.122E-01 1.168E+03  
 \*\* A2B  
 FCC  
 Calculated. 16 equilibria  
 Terminating at known equilibrium

Phase region boundary 17 at: 6.122E-01 1.168E+03  
 \*\* A2B  
 FCC  
 Calculated. 9 equilibria  
 Terminating at known equilibrium

Phase region boundary 18 at: 9.533E-01 3.100E+02  
 BCC  
 \*\* FCC  
 Calculated.. 2 equilibria  
 Terminating at axis limit.

Phase region boundary 19 at: 9.530E-01 3.000E+02  
 BCC  
 \*\* FCC  
 Calculated 31 equilibria

Phase region boundary 20 at: 9.533E-01 3.100E+02  
 BCC  
 \*\* FCC  
 Calculated 29 equilibria

Phase region boundary 21 at: 9.533E-01 3.100E+02  
 BCC  
 \*\* FCC  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 22 at: 9.533E-01 3.100E+02  
 BCC  
 \*\* FCC  
 Calculated 29 equilibria

Phase region boundary 23 at: 6.769E-02 7.700E+02  
 BCC  
 \*\* FCC  
 Calculated.. 15 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 24 at: 6.769E-02 7.700E+02  
 BCC  
 \*\* FCC  
 Calculated. 15 equilibria  
 Terminating at known equilibrium

Phase region boundary 25 at: 9.745E-01 7.700E+02  
 BCC  
 \*\* FCC  
 Calculated.. 15 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 26 at: 9.745E-01 7.700E+02  
 BCC  
 \*\* FCC  
 Calculated 18 equilibria

Phase region boundary 27 at: 1.086E-01 1.230E+03  
 BCC  
 \*\* FCC  
 Calculated.. 28 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 28 at: 1.086E-01 1.230E+03  
 BCC  
 \*\* FCC  
 Calculated. 2 equilibria  
 Terminating at known equilibrium

Phase region boundary 29 at: 8.359E-01 1.230E+03  
 \*\* LIQUID  
 FCC  
 Calculated. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 30 at: 8.359E-01 1.230E+03  
 \*\* LIQUID  
 FCC  
 Calculated 37 equilibria

Phase region boundary 31 at: 6.124E-03 1.396E+03  
 LIQUID  
 \*\* BCC  
 Calculated 11 equilibria

Phase region boundary 32 at: 6.124E-03 1.396E+03  
 LIQUID  
 \*\* BCC  
 Calculated. 9 equilibria  
 Terminating at known equilibrium

Phase region boundary 33 at: 2.658E-01 1.244E+03  
 LIQUID  
 \*\* FCC  
 Calculated. 2 equilibria  
 Terminating at known equilibrium

Phase region boundary 34 at: 2.658E-01 1.244E+03  
 LIQUID  
 \*\* FCC  
 Calculated. 5 equilibria

Terminating at known equilibrium

Phase region boundary 35 at: 6.122E-01 1.246E+03

LIQUID

\*\* A2B

Calculated. 13 equilibria

Terminating at known equilibrium

Phase region boundary 36 at: 6.122E-01 1.246E+03

LIQUID

\*\* A2B

Calculated. 4 equilibria

Terminating at known equilibrium

Phase region boundary 37 at: 9.944E-01 1.601E+03

LIQUID

\*\* FCC

Calculated. 33 equilibria

Terminating at known equilibrium

Phase region boundary 38 at: 9.944E-01 1.601E+03

LIQUID

\*\* FCC

Calculated 12 equilibria

\*\*\* BUFFER SAVED ON FILE:

c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tce  
x36.POLY3

CPU time for mapping 0 seconds

POLY\_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-l d

... the command in full is SET\_LABEL\_CURVE\_OPTION

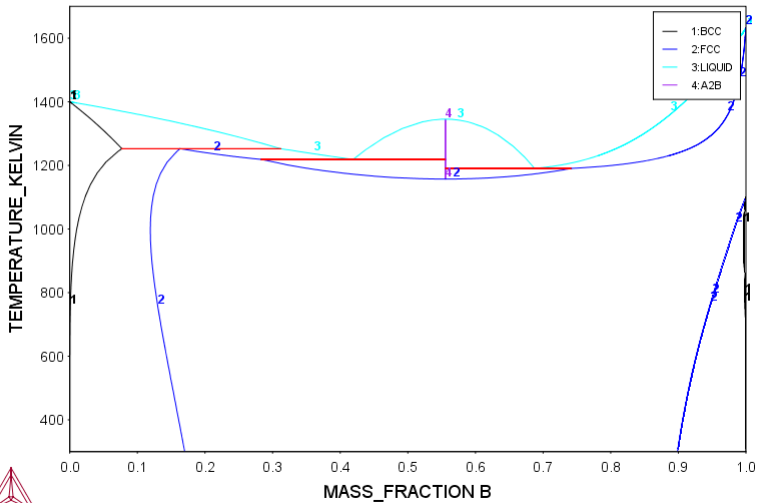
POST: plot

... the command in full is PLOT DIAGRAM

2016.05.16.14.20.12

UNKNOWN: A,B

P=1E5,N=1



POST:

POST: set-inter

... the command in full is SET\_INTERACTIVE\_MODE

POST:Hit RETURN to continue

POST: ba

... the command in full is BACK

POLY\_3: ba

... the command in full is BACK

PARROT VERSION 5.3

Global minimization used as test only

PARROT: @@ This does not look very good, optimize more ...

PARROT: opt 30

... the command in full is OPTIMIZE\_VARIABLES

Alternate calculation is on

Use 47 experiments, maximum is 2000

Use 824 real workspace, maximum is 50000

The following output is provided by subroutine VA05A

AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 9.80059382E-01  
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00  
6 1.0000E+00 7 1.0000E+00

AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 9.80052014E-01  
1 1.0001E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00  
6 1.0000E+00 7 1.0000E+00

AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 9.80051985E-01  
1 1.0001E+00 2 1.0001E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00  
6 1.0000E+00 7 1.0000E+00

AT THE 3 RD ITERATION WE HAVE THE SUM OF SQUARES 9.79978216E-01  
1 1.0001E+00 2 1.0001E+00 3 1.0001E+00 4 1.0000E+00 5 1.0000E+00  
6 1.0000E+00 7 1.0000E+00

AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 9.79978097E-01  
1 1.0001E+00 2 1.0001E+00 3 1.0001E+00 4 1.0001E+00 5 1.0000E+00  
6 1.0000E+00 7 1.0000E+00

AT THE 5 TH ITERATION WE HAVE THE SUM OF SQUARES 9.79978348E-01  
1 1.0001E+00 2 1.0001E+00 3 1.0001E+00 4 1.0001E+00 5 1.0001E+00

```

6 1.0000E+00 7 1.0000E+00

      AT THE 6 TH ITERATION WE HAVE THE SUM OF SQUARES 9.80052308E-01
1 1.0001E+00 2 1.0001E+00 3 1.0001E+00 4 1.0001E+00 5 1.0000E+00
6 1.0001E+00 7 1.0000E+00

      AT THE 7 TH ITERATION WE HAVE THE SUM OF SQUARES 9.79979005E-01
1 1.0001E+00 2 1.0001E+00 3 1.0001E+00 4 1.0001E+00 5 1.0000E+00
6 1.0000E+00 7 1.0001E+00

      AT THE 8 TH ITERATION WE HAVE THE SUM OF SQUARES 9.74568992E-01
1 1.0007E+00 2 1.0001E+00 3 1.0074E+00 4 1.0001E+00 5 9.9998E-01
6 9.9266E-01 7 1.0000E+00

      AT THE 9 TH ITERATION WE HAVE THE SUM OF SQUARES 9.68323516E-01
1 1.0001E+00 2 9.9993E-01 3 1.0086E+00 4 1.0048E+00 5 9.9962E-01
6 9.8903E-01 7 9.9159E-01

      AT THE 10 TH ITERATION WE HAVE THE SUM OF SQUARES 9.58298224E-01
1 1.0012E+00 2 9.9951E-01 3 1.0105E+00 4 1.0150E+00 5 9.9882E-01
6 9.7286E-01 7 9.8384E-01

      AT THE 11 TH ITERATION WE HAVE THE SUM OF SQUARES 9.36475670E-01
1 9.9970E-01 2 9.9934E-01 3 1.0140E+00 4 1.0400E+00 5 9.9747E-01
6 9.4967E-01 7 9.6043E-01

      AT THE 12 TH ITERATION WE HAVE THE SUM OF SQUARES 8.96558227E-01
1 1.0019E+00 2 9.9883E-01 3 1.0209E+00 4 1.0903E+00 5 9.9477E-01
6 8.9661E-01 7 9.2172E-01

      AT THE 13 TH ITERATION WE HAVE THE SUM OF SQUARES 8.20182625E-01
1 9.9941E-01 2 9.9846E-01 3 1.0352E+00 4 1.1942E+00 5 9.8966E-01
6 7.9747E-01 7 8.3959E-01

      AT THE 14 TH ITERATION WE HAVE THE SUM OF SQUARES 6.87461582E-01
1 1.0018E+00 2 9.9752E-01 3 1.0636E+00 4 1.4027E+00 5 9.7946E-01
6 5.9608E-01 7 6.7987E-01

      AT THE 15 TH ITERATION WE HAVE THE SUM OF SQUARES 6.87514987E-01
1 1.0019E+00 2 9.9752E-01 3 1.0636E+00 4 1.4027E+00 5 9.7946E-01
6 5.9609E-01 7 6.7985E-01

      AT THE 16 TH ITERATION WE HAVE THE SUM OF SQUARES 6.87460994E-01
1 1.0018E+00 2 9.9762E-01 3 1.0636E+00 4 1.4027E+00 5 9.7946E-01
6 5.9608E-01 7 6.7987E-01

      AT THE 17 TH ITERATION WE HAVE THE SUM OF SQUARES 4.93890786E-01
1 9.9983E-01 2 9.9617E-01 3 1.1210E+00 4 1.8222E+00 5 9.5929E-01
6 1.9649E-01 7 3.5984E-01

      AT THE 18 TH ITERATION WE HAVE THE SUM OF SQUARES 3.83968704E-01
1 1.0003E+00 2 9.9394E-01 3 1.2080E+00 4 2.4586E+00 5 9.2882E-01
6 -4.0863E-01 7 -1.2364E-01

      THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 18 iterations
1 1.0003E+00 2 9.9394E-01 3 1.2080E+00 4 2.4586E+00 5 9.2882E-01
6 -4.0863E-01 7 -1.2364E-01

1 5.6826E-03 2 5.6826E-03 3 -5.2705E-04 4 -1.0121E-03 5 1.2997E-01
6 -1.3615E-01 7 9.2250E-04 8 5.4224E-03 9 5.4224E-03 10 5.3339E-04
11 -6.9115E-03 12 2.1376E-03 13 -5.6501E-03 14 2.0876E-03 15 -5.3921E-03
16 9.5282E-03 17 9.5282E-03 18 2.1204E-04 19 -3.0973E-03 20 2.1204E-04
21 -3.0973E-03 22 -2.1113E-03 23 -3.4457E-04 24 3.5839E-03 25 -3.0619E-03
26 -3.2846E-03 27 -2.5884E-03 28 -6.7137E-04 29 -4.9774E-03 30 2.1227E-03
31 2.5569E-02 32 1.1253E-01 33 2.1861E-01 34 2.9732E-01 35 3.0190E-01
36 1.8750E-01 37 2.4843E-01 38 9.3003E-02 39 1.7059E-03 40 1.9922E-02
41 1.4647E-02 42 7.8823E-03 43 1.6274E-03 44 -4.1177E-03 45 -1.1353E-02
46 -1.8078E-02 47 -2.6294E-02

      THE SUM OF SQUARES IS 3.83968704E-01

PARROT: resc
... the command in full is RESCALE_VARIABLES
PARROT: opt 30
... the command in full is OPTIMIZE_VARIABLES
Alternate calculation is on
Use 47 experiments, maximum is 2000
Use 824 real workspace, maximum is 50000
The following output is provided by subroutine VA05A

      AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 3.83968704E-01
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00

      AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 3.83970580E-01
1 1.0001E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00

      AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 3.83968793E-01
1 1.0000E+00 2 1.0001E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00

      AT THE 3 RD ITERATION WE HAVE THE SUM OF SQUARES 3.83969329E-01
1 1.0000E+00 2 1.0000E+00 3 1.0001E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00

      AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 3.83968753E-01
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0001E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00

      AT THE 5 TH ITERATION WE HAVE THE SUM OF SQUARES 3.83968710E-01
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0001E+00
6 1.0000E+00 7 1.0000E+00

      AT THE 6 TH ITERATION WE HAVE THE SUM OF SQUARES 3.83968800E-01
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0001E+00 7 1.0000E+00

      AT THE 7 TH ITERATION WE HAVE THE SUM OF SQUARES 3.83968718E-01
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0001E+00

      THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 7 iterations
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00

```

```

1 5.6826E-03 2 5.6826E-03 3 -5.2705E-04 4 -1.0121E-03 5 1.2997E-01
6 -1.3615E-01 7 9.2250E-04 8 5.4224E-03 9 5.4224E-03 10 5.3339E-04
11 -6.9115E-03 12 2.1376E-03 13 -5.6501E-03 14 2.0876E-03 15 -5.3921E-03
16 9.5282E-03 17 9.5282E-03 18 2.1204E-04 19 -3.0973E-03 20 2.1204E-04
21 -3.0973E-03 22 -2.1113E-03 23 -3.4457E-04 24 3.5839E-03 25 -3.0619E-03
26 -3.2846E-03 27 -2.5884E-03 28 -6.7137E-04 29 -4.9774E-03 30 2.1227E-03
31 2.5569E-02 32 1.1253E-01 33 2.1861E-01 34 2.9732E-01 35 3.0190E-01
36 1.8750E-01 37 2.4843E-01 38 9.3003E-02 39 1.7059E-03 40 1.9922E-02
41 1.4647E-02 42 7.8823E-03 43 1.6274E-03 44 -4.1177E-03 45 -1.1353E-02
46 -1.8078E-02 47 -2.6294E-02

```

THE SUM OF SQUARES IS 3.83968704E-01

PARROT: @@ No change in the parameters, check the diagram again

PARROT: mac tcex36cpd

... the command in full is MACRO\_FILE\_OPEN

PARROT: set-echo

NO SUCH COMMAND, USE HELP

PARROT: @@ Calculate the phase diagram

PARROT: @@ This TCM should be run in PARROT

PARROT: go p-3

... the command in full is GOTO\_MODULE

POLY\_3:

POLY\_3: @@ In PARROT, the global minimization is turned off automatically.

POLY\_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning

POLY\_3: @@ message will be given.

POLY\_3:

POLY\_3: advanced-option global yes,,

... the command in full is ADVANCED\_OPTIONS

Settings for global minimization:

\*\*\* WARNING \*\*\* Global equilibrium calculation may create new composition sets

and this may corrupt your PARROT work file (.PAR file).

Do not go back to PARROT but exit from POLY after your POLY calculations.

POLY\_3:

POLY\_3: def-com,,,,

... the command in full is DEFINE\_COMPONENTS

POLY\_3: s-a-v 1 w(b) 0 1,,,,

... the command in full is SET\_AXIS\_VARIABLE

The condition W(B)=.1234 created

POLY\_3: s-a-v 2 t 300 1700,,,,

... the command in full is SET\_AXIS\_VARIABLE

The condition T=942.2 created

POLY\_3: s-c t=500

... the command in full is SET\_CONDITION

POLY\_3: l-c

... the command in full is LIST\_CONDITIONS

W(B)=0.1234, P=1E5, N=1, T=500

DEGREES OF FREEDOM 0

POLY\_3: c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Using global minimization procedure

Calculated 412 grid points in 0 s

Found the set of lowest grid points in 0 s

Calculated POLY solution 0 s, total time 0 s

POLY\_3: save tcex36 y

... the command in full is SAVE\_WORKSPACES

This file contains results from a previous STEP or MAP command.

The SAVE command will save the current status of the program but destroy

the results from the previous STEP or MAP commands.

POLY\_3: map

Version 5 mapping is selected

Generating start equilibrium 1

Generating start equilibrium 2

Generating start equilibrium 3

Generating start equilibrium 4

Generating start equilibrium 5

Generating start equilibrium 6

Generating start equilibrium 7

Generating start equilibrium 8

Generating start equilibrium 9

Generating start equilibrium 10

Generating start equilibrium 11

Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1

Generating start point 2

Generating start point 3

Generating start point 4

Generating start point 5

Generating start point 6

Generating start point 7

Generating start point 8

Generating start point 9

Generating start point 10

Working hard

Generating start point 11

Generating start point 12

Generating start point 13

Generating start point 14

Generating start point 15

Generating start point 16

Generating start point 17

Generating start point 18

Generating start point 19

Generating start point 20

Working hard

Generating start point 21

Generating start point 22

Generating start point 23

Generating start point 24

Generating start point 25

Generating start point 26

Generating start point 27

Generating start point 28

Phase region boundary 1 at: 7.140E-01 3.100E+02

BCC

\*\* BCC#2

Calculated.. 2 equilibria

Terminating at axis limit.

Phase region boundary 2 at: 7.141E-01 3.000E+02  
 BCC  
 \*\* BCC#2  
 Calculated. 14 equilibria

Phase region boundary 3 at: 6.802E-01 7.347E+02  
 \*\* A2B  
 BCC  
 \*\* BCC#2

Phase region boundary 4 at: 3.640E-01 7.347E+02  
 \*\* A2B  
 BCC  
 Calculated. 14 equilibria

Phase region boundary 5 at: 3.781E-01 1.187E+03  
 \*\* LIQUID  
 \*\* A2B  
 BCC

Phase region boundary 6 at: 2.888E-01 1.187E+03  
 \*\* LIQUID  
 BCC  
 Calculated 27 equilibria

Phase region boundary 7 at: 4.898E-01 1.187E+03  
 \*\* LIQUID  
 A2B  
 Calculated. 26 equilibria

Phase region boundary 8 at: 6.479E-01 1.047E+03  
 \*\* LIQUID  
 A2B  
 \*\* BCC

Phase region boundary 9 at: 7.629E-01 1.047E+03  
 A2B  
 \*\* BCC  
 Calculated. 10 equilibria  
 Terminating at known equilibrium

Phase region boundary 10 at: 8.250E-01 1.047E+03  
 LIQUID  
 \*\* BCC  
 Calculated. 9 equilibria

Phase region boundary 11 at: 8.738E-01 1.205E+03  
 LIQUID  
 \*\* BCC  
 \*\* FCC

Phase region boundary 12 at: 8.791E-01 1.205E+03  
 LIQUID  
 \*\* FCC  
 Calculated 37 equilibria

Phase region boundary 13 at: 9.347E-01 1.205E+03  
 BCC  
 \*\* FCC  
 Calculated 26 equilibria

Phase region boundary 14 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated. 14 equilibria  
 Terminating at known equilibrium

Phase region boundary 15 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 16 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated. 14 equilibria  
 Terminating at known equilibrium

Phase region boundary 17 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 18 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated. 14 equilibria  
 Terminating at known equilibrium

Phase region boundary 19 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 20 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated. 14 equilibria  
 Terminating at known equilibrium

Phase region boundary 21 at: 7.140E-01 3.100E+02  
 \*\* BCC  
 BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 22 at: 7.140E-01 3.100E+02  
 \*\* BCC

BCC#2  
 Calculated. 14 equilibria  
 Terminating at known equilibrium  
 Phase region boundary 23 at: 7.140E-01 3.100E+02  
 \*\* BCC  
 BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.  
 Phase region boundary 24 at: 7.140E-01 3.100E+02  
 \*\* BCC  
 BCC#2  
 Calculated. 14 equilibria  
 Terminating at known equilibrium  
 Phase region boundary 25 at: 3.657E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated 10 equilibria  
 Phase region boundary 26 at: 3.657E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated. 3 equilibria  
 Terminating at known equilibrium  
 Phase region boundary 27 at: 3.657E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated. 13 equilibria  
 Terminating at known equilibrium  
 Phase region boundary 28 at: 7.900E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated 10 equilibria  
 Phase region boundary 29 at: 7.900E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated. 3 equilibria  
 Terminating at known equilibrium  
 Phase region boundary 30 at: 7.900E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated. 9 equilibria  
 Terminating at known equilibrium  
 Phase region boundary 31 at: 2.459E-01 1.230E+03  
 \*\* LIQUID  
 BCC  
 Calculated. 4 equilibria  
 Terminating at known equilibrium  
 Phase region boundary 32 at: 2.459E-01 1.230E+03  
 \*\* LIQUID  
 BCC  
 Calculated 26 equilibria  
 Phase region boundary 33 at: 8.847E-01 1.230E+03  
 \*\* LIQUID  
 FCC  
 Calculated. 2 equilibria  
 Terminating at known equilibrium  
 Phase region boundary 34 at: 8.847E-01 1.230E+03  
 \*\* LIQUID  
 FCC  
 Calculated 29 equilibria  
 Phase region boundary 35 at: 6.422E-03 1.397E+03  
 LIQUID  
 \*\* BCC  
 Calculated 9 equilibria  
 Phase region boundary 36 at: 6.422E-03 1.397E+03  
 LIQUID  
 \*\* BCC  
 Calculated. 13 equilibria  
 Terminating at known equilibrium  
 Phase region boundary 37 at: 2.299E-01 1.244E+03  
 LIQUID  
 \*\* BCC  
 Calculated 19 equilibria  
 Phase region boundary 38 at: 2.299E-01 1.244E+03  
 LIQUID  
 \*\* BCC  
 Calculated. 4 equilibria  
 Terminating at known equilibrium  
 Phase region boundary 39 at: 6.122E-01 1.219E+03  
 LIQUID  
 \*\* A2B  
 Calculated. 12 equilibria  
 Terminating at known equilibrium  
 Phase region boundary 40 at: 6.122E-01 1.219E+03  
 LIQUID  
 \*\* A2B  
 Calculated. 7 equilibria  
 Terminating at known equilibrium  
 Phase region boundary 41 at: 9.927E-01 1.613E+03  
 LIQUID  
 \*\* FCC  
 Calculated. 20 equilibria  
 Terminating at known equilibrium  
 Phase region boundary 42 at: 9.927E-01 1.613E+03  
 LIQUID  
 \*\* FCC

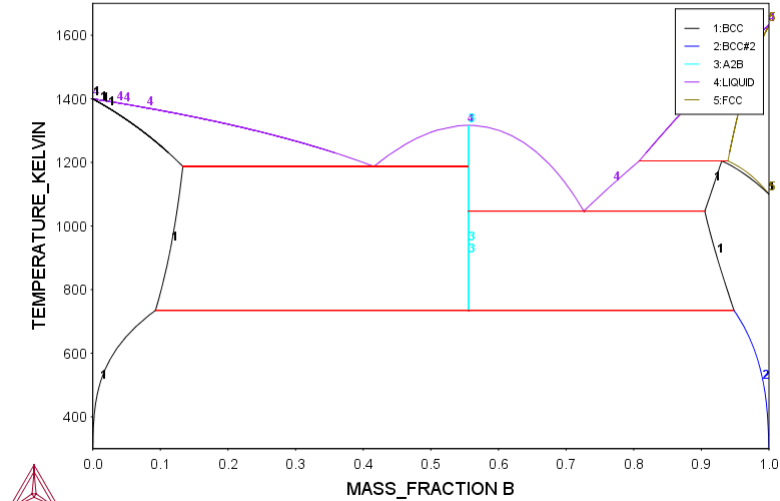


Calculated 13 equilibria  
 \*\*\* BUFFER SAVED ON FILE:  
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tce  
 x36.POLY3  
 CPU time for mapping 0 seconds  
 POLY\_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-l d  
 ... the command in full is SET\_LABEL\_CURVE\_OPTION  
 POST: plot  
 ... the command in full is PLOT DIAGRAM  
 2016.05.16.14.20.19  
 UNKNOWN: A,B  
 P=1E5,N=1



POST: set-inter  
 ... the command in full is SET\_INTERACTIVE\_MODE  
 POST:Hit RETURN to continue  
 POST: ba  
 ... the command in full is BACK  
 POLY\_3: ba  
 ... the command in full is BACK

PARROT VERSION 5.3

Global minimization used as test only  
 PARROT: @@ Turn off alternate mode and try to calculate all equilibria  
 PARROT: s-alt Y  
 ... the command in full is SET\_ALTERNATE\_MODE  
 Alternate calculation is on

PARROT: ed  
 ... the command in full is EDIT\_EXPERIMENTS  
 ED\_EXP: read 1  
 ... the command in full is READ\_WORKSPACES

ED\_EXP: c-a  
 ... the command in full is COMPUTE\_ALL\_EQUILIBRIA

Eq	Lab	Iter	Weight	Temp	Exp	Fix phases or comments
1	AINV	3	1.	1187.5		LIQUID A2B BCC
2	AINV	2	1.	1316.7		LIQUID A2B
3	AINV	3	1.	1047.0		LIQUID A2B BCC
4	AINV	3	1.	1204.7		LIQUID BCC FCC
5	AINV	4	1.	734.7		A2B BCC BCC#2
6	AINV	3	1.	726.0		BCC BCC#2
10	ALF	< unused >		1594.0		LIQUID FCC
11	ALF	< unused >		1548.0		LIQUID FCC
12	ALF	< unused >		1499.0		LIQUID FCC
13	ALF	< unused >		1438.0		LIQUID FCC
20	ATIE	3	1.	1413.0		LIQUID FCC
21	ATIE	3	1.	1337.0		LIQUID FCC
22	ATIE	3	1.	1213.0		LIQUID FCC
23	ATIE	3	1.	1100.0		LIQUID BCC
100	AA	2	1.	1573.0		LIQUID
101	AA	2	1.	1573.0		LIQUID
102	AA	2	1.	1573.0		LIQUID
103	AA	2	1.	1573.0		LIQUID
104	AA	2	1.	1573.0		LIQUID
105	AA	2	1.	1573.0		LIQUID
106	AA	2	1.	1573.0		LIQUID
107	AA	2	1.	1573.0		LIQUID
108	AA	2	1.	1573.0		LIQUID
110	AH	2	1.	1773.0		LIQUID
111	AH	2	1.	1773.0		LIQUID
112	AH	2	1.	1773.0		LIQUID
113	AH	2	1.	1773.0		LIQUID
114	AH	2	1.	1773.0		LIQUID
115	AH	2	1.	1773.0		LIQUID
116	AH	2	1.	1773.0		LIQUID
117	AH	2	1.	1773.0		LIQUID
118	AH	2	1.	1773.0		LIQUID

ED\_EXP: @@ Remove the equilibria with just liquid as we do not optimize  
 ED\_EXP: @@ any liquid parameters and restore those with label ALF  
 ED\_EXP: s-we 0 100-118  
 ... the command in full is SET\_WEIGHT  
 ED\_EXP: s-we 1 alf  
 ... the command in full is SET\_WEIGHT  
 Changed weight on 4 equilibria.  
 ED\_EXP: s-e 1  
 ... the command in full is SELECT\_EQUILIBRIUM  
 Equilibrium number 1, label AINV  
 ED\_EXP: c-a

```

... the command in full is COMPUTE_ALL_EQUILIBRIA
Eq Lab Iter Weight Temp Exp Fix phases or comments
1 AINV 2 1. 1187.5 LIQUID A2B BCC
2 AINV 2 1. 1316.7 LIQUID A2B
3 AINV 2 1. 1047.0 LIQUID A2B BCC
4 AINV 2 1. 1204.7 LIQUID BCC FCC
5 AINV 2 1. 734.7 A2B BCC BCC#2
6 AINV 2 1. 726.0 BCC BCC#2
10 ALF 6 1. 1594.0 LIQUID FCC
11 ALF 6 1. 1548.0 LIQUID FCC
12 ALF 7 1. 1499.0 LIQUID FCC
13 ALF 7 1. 1438.0 LIQUID FCC
20 ATIE 2 1. 1413.0 LIQUID FCC
21 ATIE 2 1. 1337.0 LIQUID FCC
22 ATIE 2 1. 1213.0 LIQUID FCC
23 ATIE 2 1. 1100.0 LIQUID BCC
100 AA < unused > 1573.0 LIQUID
101 AA < unused > 1573.0 LIQUID
102 AA < unused > 1573.0 LIQUID
103 AA < unused > 1573.0 LIQUID
104 AA < unused > 1573.0 LIQUID
105 AA < unused > 1573.0 LIQUID
106 AA < unused > 1573.0 LIQUID
107 AA < unused > 1573.0 LIQUID
108 AA < unused > 1573.0 LIQUID
110 AH < unused > 1773.0 LIQUID
111 AH < unused > 1773.0 LIQUID
112 AH < unused > 1773.0 LIQUID
113 AH < unused > 1773.0 LIQUID
114 AH < unused > 1773.0 LIQUID
115 AH < unused > 1773.0 LIQUID
116 AH < unused > 1773.0 LIQUID
117 AH < unused > 1773.0 LIQUID
118 AH < unused > 1773.0 LIQUID

```

ED\_EXP: save

... the command in full is SAVE\_WORKSPACES

ED\_EXP: @@ Save changes

ED\_EXP: ba

... the command in full is BACK

PARROT: opt 0

... the command in full is OPTIMIZE\_VARIABLES

Use 29 experiments, maximum is 2000

Use 554 real workspace, maximum is 50000

PARROT: l-r C SCREEN

... the command in full is LIST\_RESULT

```

=====
OUTPUT FROM P A R R O T. DATE 2016. 5.16 14:20:20

```

\*\*\* SUCCESSFUL OPTIMIZATION. \*\*\*  
NUMBER OF ITERATIONS: 0

== OPTIMIZING CONDITIONS ==

```

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 0 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

```

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.02757864E+04	2.02757864E+04	2.02757864E+04	7.39333291E-02
V2	-2.90134088E+01	-2.90134088E+01	-2.90134088E+01	3.44753302E-01
V11	-2.18127452E+04			
V12	1.55559572E+01			
V15	2.39869483E+04	2.39869483E+04	2.39869483E+04	6.19220768E-01
V16	-8.02178633E+00	-8.02178633E+00	-8.02178633E+00	2.18789658E+00
V17	3.13540526E+03	3.13540526E+03	3.13540526E+03	1.44882543E+00
V19	2.12643554E+04	2.12643554E+04	2.12643554E+04	4.78622311E+00
V20	-6.23643289E+00	-6.23643289E+00	-6.23643289E+00	1.26469088E+01

```

NUMBER OF OPTIMIZING VARIABLES : 7
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 3.83968704E-01 TO 7.41792272E+00
DEGREES OF FREEDOM 22. REDUCED SUM OF SQUARES 3.37178306E-01

```

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS

DX=2E-2, P0=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%

HTR=HM(LIQUID)-HM(A2B)

1 T=1193	1187.	10.0	-5.532	-0.5532
1 W(LIQUID,B)=0.408	0.4157	2.00E-02	7.7215E-03	0.3861
1 W(BCC,B)=0.13	0.1332	2.00E-02	3.2119E-03	0.1606
2 T=1341	1317.	10.0	-24.32	-2.432
2 HTR=3727	3727.	5.00E+02	0.4611	9.2229E-04
3 T=1049	1047.	10.0	-1.990	-0.1990
3 W(LIQUID,A)=0.27	0.2739	2.00E-02	3.9062E-03	0.1953
3 W(BCC,A)=9.3E-2	9.4971E-02	2.00E-02	1.9713E-03	9.8563E-02
4 T=1203	1205.	10.0	1.671	0.1671
4 W(LIQUID,A)=0.19	0.1919	2.00E-02	1.8666E-03	9.3330E-02
4 W(BCC,A)=6.9E-2	6.9780E-02	2.00E-02	7.8014E-04	3.9007E-02
4 W(FCC,A)=6E-2	6.0794E-02	2.00E-02	7.9445E-04	3.9723E-02
5 T=726	734.7	10.0	8.703	0.8703
5 X(BCC,B)=3.7E-2	3.9289E-02	2.00E-02	2.2886E-03	0.1144
5 X(BCC#2,A)=0.114	0.1200	2.00E-02	6.0001E-03	0.3000
6 X(BCC,B)=3.7E-2	3.6833E-02	2.00E-02	-1.6665E-04	-8.3327E-03
6 X(BCC#2,A)=0.114	0.1140	2.00E-02	-1.6829E-05	-8.4144E-04
10 W(LIQUID,A)=2E-2	1.9506E-02	2.00E-02	-4.9427E-04	-2.4713E-02

11 W(LIQUID,A)=4.2E-2	4.1827E-02	2.00E-02	-1.7330E-04	-8.6648E-03
12 W(LIQUID,A)=6.5E-2	6.5040E-02	2.00E-02	4.0133E-05	2.0066E-03
13 W(LIQUID,A)=9.3E-2	9.3114E-02	2.00E-02	1.1416E-04	5.7082E-03
20 W(LIQUID,A)=0.104	0.1043	2.00E-02	3.4980E-04	1.7490E-02
20 W(FCC,A)=3.8E-2	3.8244E-02	2.00E-02	2.4396E-04	1.2198E-02
21 W(LIQUID,A)=0.136	0.1375	2.00E-02	1.5284E-03	7.6418E-02
21 W(FCC,A)=4.7E-2	4.7395E-02	2.00E-02	3.9496E-04	1.9748E-02
22 W(LIQUID,A)=0.187	0.1886	2.00E-02	1.5692E-03	7.8460E-02
22 W(FCC,A)=5.9E-2	6.0019E-02	2.00E-02	1.0194E-03	5.0968E-02
23 W(LIQUID,A)=0.245	0.2474	2.00E-02	2.3699E-03	0.1185
23 W(BCC,A)=8.5E-2	8.6337E-02	2.00E-02	1.3367E-03	6.6834E-02

```

PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ When we optimize zero times we sometimes find an error for equilibrium 4
PARROT: @@ It can be on the wrong side, at high A instead of high B. Try to correct
PARROT: @@ that in the edit module.
PARROT: ed
... the command in full is EDIT_EXPERIMENTS
ED_EXP: read 1
... the command in full is READ_WORKSPACES
ED_EXP: s-e 4
... the command in full is SELECT_EQUILIBRIUM
Equilibrium number      4 , label AINV
ED_EXP: s-a-s
... the command in full is SET_ALL_START_VALUES
T /1204.671469/: 1200
Automatic start values for phase constituents? /N/: N

Phase LIQUID
Major constituent(s) /*/: b

Phase BCC
Major constituent(s) /b/: b

Phase FCC
Major constituent(s) /b/: b
ED_EXP:
ED_EXP: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Testing result with global minimization
14 ITS, CPU TIME USED 0 SECONDS
ED_EXP: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
Output from POLY-3, equilibrium =      4, label AINV, database: UNKNOWN

Conditions:
P=1.01325E5
FIXED PHASES
LIQUID=1 BCC=1 FCC=1
DEGREES OF FREEDOM 0

Temperature 1204.67 K ( 931.52 C), Pressure 1.013250E+05
Number of moles of components 3.00000E+00, Mass in grams 1.29910E+02
Total Gibbs energy -9.73780E+03, Enthalpy 1.97627E+04, Volume 0.00000E+00

Component      Moles      W-Fraction Activity Potential Ref.stat
A      6.6968E-01  1.0310E-01 4.0116E-01 -9.1489E+03 SER
B      2.3303E+00  8.9690E-01 8.5667E-01 -1.5496E+03 SER

FCC      Status FIXED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 4.5821E+01, Volume fraction 0.0000E+00 Mass fractions:
B 9.39206E-01 A 6.07945E-02

BCC      Status FIXED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 4.5262E+01, Volume fraction 0.0000E+00 Mass fractions:
B 9.30220E-01 A 6.97801E-02

LIQUID      Status FIXED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 3.8826E+01, Volume fraction 0.0000E+00 Mass fractions:
B 8.08133E-01 A 1.91867E-01

EXPERIMENT T=1203:DT $1204.67:10 NO=1
EXPERIMENT W(LIQUID,A)=0.19:DX $0.191867:2E-2 NO=2
EXPERIMENT W(BCC,A)=6.9E-2:DX $6.97801E-2:2E-2 NO=3
EXPERIMENT W(FCC,A)=6E-2:DX $6.07945E-2:2E-2 NO=4
ED_EXP: ba
... the command in full is BACK
PARROT: @@ The error is still there, calculate the phase diagram!!!
PARROT: mac tcex36cpd
... the command in full is MACRO_FILE_OPEN
PARROT: set-echo
NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
... the command in full is GOTO_MODULE
POLY_3:
POLY_3: @@ In PARROT, the global minimization is turned off automatically.
POLY_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY_3: @@ message will be given.
POLY_3:
POLY_3: advanced-option global yes,,
... the command in full is ADVANCED_OPTIONS
Settings for global minimization:
*** WARNING *** Global equilibrium calculation may create new composition sets
and this may corrupt your PARROT work file (.PAR file).
Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY_3:
POLY_3: def-com,,,,
... the command in full is DEFINE_COMPONENTS
POLY_3: s-a-v 1 w(b) 0 1,,,,
... the command in full is SET_AXIS_VARIABLE
The condition W(B)=.1234 created
POLY_3: s-a-v 2 t 300 1700,,,,
... the command in full is SET_AXIS_VARIABLE
The condition T=942.2 created
POLY_3: s-c t=500
... the command in full is SET_CONDITION
POLY_3: l-c
... the command in full is LIST_CONDITIONS

```

W(B)=0.1234, P=1E5, N=1, T=500  
DEGREES OF FREEDOM 0

**POLY\_3:** c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Using global minimization procedure

Calculated 412 grid points in 0 s

Found the set of lowest grid points in 0 s

Calculated POLY solution 1 s, total time 1 s

**POLY\_3:** save tcex36 y

... the command in full is SAVE\_WORKSPACES

This file contains results from a previous STEP or MAP command.

The SAVE command will save the current status of the program but destroy the results from the previous STEP or MAP commands.

**POLY\_3:** map

Version S mapping is selected

Generating start equilibrium 1

Generating start equilibrium 2

Generating start equilibrium 3

Generating start equilibrium 4

Generating start equilibrium 5

Generating start equilibrium 6

Generating start equilibrium 7

Generating start equilibrium 8

Generating start equilibrium 9

Generating start equilibrium 10

Generating start equilibrium 11

Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1

Generating start point 2

Generating start point 3

Generating start point 4

Generating start point 5

Generating start point 6

Generating start point 7

Generating start point 8

Generating start point 9

Generating start point 10

Working hard

Generating start point 11

Generating start point 12

Generating start point 13

Generating start point 14

Generating start point 15

Generating start point 16

Generating start point 17

Generating start point 18

Generating start point 19

Generating start point 20

Working hard

Generating start point 21

Generating start point 22

Generating start point 23

Generating start point 24

Generating start point 25

Generating start point 26

Generating start point 27

Generating start point 28

Phase region boundary 1 at: 7.140E-01 3.100E+02

BCC

\*\* BCC#2

Calculated.. 2 equilibria

Terminating at axis limit.

Phase region boundary 2 at: 7.141E-01 3.000E+02

BCC

\*\* BCC#2

Calculated. 14 equilibria

Phase region boundary 3 at: 6.802E-01 7.347E+02

\*\* A2B

BCC

\*\* BCC#2

Phase region boundary 4 at: 3.640E-01 7.347E+02

\*\* A2B

BCC

Calculated. 14 equilibria

Phase region boundary 5 at: 3.781E-01 1.187E+03

\*\* LIQUID

\*\* A2B

BCC

Phase region boundary 6 at: 2.888E-01 1.187E+03

\*\* LIQUID

BCC

Calculated 27 equilibria

Phase region boundary 7 at: 4.898E-01 1.187E+03

\*\* LIQUID

A2B

Calculated. 26 equilibria

Phase region boundary 8 at: 6.479E-01 1.047E+03

\*\* LIQUID

A2B

\*\* BCC

Phase region boundary 9 at: 7.629E-01 1.047E+03

A2B

\*\* BCC

Calculated. 10 equilibria

Terminating at known equilibrium

Phase region boundary 10 at: 8.250E-01 1.047E+03

LIQUID

\*\* BCC

Calculated. 9 equilibria

Phase region boundary 11 at: 8.738E-01 1.205E+03  
 LIQUID  
 \*\* BCC  
 \*\* FCC

Phase region boundary 12 at: 8.791E-01 1.205E+03  
 LIQUID  
 \*\* FCC  
 Calculated 37 equilibria

Phase region boundary 13 at: 9.347E-01 1.205E+03  
 BCC  
 \*\* FCC  
 Calculated 26 equilibria

Phase region boundary 14 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated. 14 equilibria  
 Terminating at known equilibrium

Phase region boundary 15 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 16 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated. 14 equilibria  
 Terminating at known equilibrium

Phase region boundary 17 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 18 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated. 14 equilibria  
 Terminating at known equilibrium

Phase region boundary 19 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 20 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated. 14 equilibria  
 Terminating at known equilibrium

Phase region boundary 21 at: 7.140E-01 3.100E+02  
 \*\* BCC  
 BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 22 at: 7.140E-01 3.100E+02  
 \*\* BCC  
 BCC#2  
 Calculated. 14 equilibria  
 Terminating at known equilibrium

Phase region boundary 23 at: 7.140E-01 3.100E+02  
 \*\* BCC  
 BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 24 at: 7.140E-01 3.100E+02  
 \*\* BCC  
 BCC#2  
 Calculated. 14 equilibria  
 Terminating at known equilibrium

Phase region boundary 25 at: 3.657E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated 10 equilibria

Phase region boundary 26 at: 3.657E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated. 3 equilibria  
 Terminating at known equilibrium

Phase region boundary 27 at: 3.657E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 28 at: 7.900E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated 10 equilibria

Phase region boundary 29 at: 7.900E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated. 3 equilibria  
 Terminating at known equilibrium

Phase region boundary 30 at: 7.900E-01 7.700E+02

```

** A2B
  BCC
Calculated.          9 equilibria
Terminating at known equilibrium

Phase region boundary 31 at:  2.459E-01  1.230E+03
** LIQUID
  BCC
Calculated.          4 equilibria
Terminating at known equilibrium

Phase region boundary 32 at:  2.459E-01  1.230E+03
** LIQUID
  BCC
Calculated          26 equilibria

Phase region boundary 33 at:  8.847E-01  1.230E+03
** LIQUID
  FCC
Calculated.          2 equilibria
Terminating at known equilibrium

Phase region boundary 34 at:  8.847E-01  1.230E+03
** LIQUID
  FCC
Calculated          29 equilibria

Phase region boundary 35 at:  6.422E-03  1.397E+03
  LIQUID
** BCC
Calculated          9 equilibria

Phase region boundary 36 at:  6.422E-03  1.397E+03
  LIQUID
** BCC
Calculated.         13 equilibria
Terminating at known equilibrium

Phase region boundary 37 at:  2.299E-01  1.244E+03
  LIQUID
** BCC
Calculated          19 equilibria

Phase region boundary 38 at:  2.299E-01  1.244E+03
  LIQUID
** BCC
Calculated.          4 equilibria
Terminating at known equilibrium

Phase region boundary 39 at:  6.122E-01  1.219E+03
  LIQUID
** A2B
Calculated.         12 equilibria
Terminating at known equilibrium

Phase region boundary 40 at:  6.122E-01  1.219E+03
  LIQUID
** A2B
Calculated.          7 equilibria
Terminating at known equilibrium

Phase region boundary 41 at:  9.927E-01  1.613E+03
  LIQUID
** FCC
Calculated.         20 equilibria
Terminating at known equilibrium

Phase region boundary 42 at:  9.927E-01  1.613E+03
  LIQUID
** FCC
Calculated          13 equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tce
x36.POLY3
CPU time for mapping          0 seconds
POLY_3: post

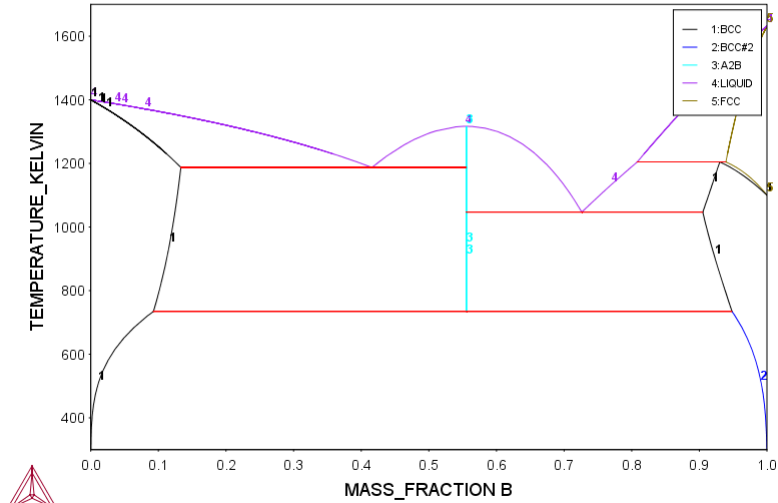
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-l d
... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
... the command in full is PLOT_DIAGRAM

```

2016.05.16.14.20.24  
A, B  
P=1E5, N=1



```

POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:Hit RETURN to continue
POST: @@ The phase diagram shows there is no equilibrium between liquid,
POST: @@ fcc and bcc at high B content. For the moment we better remove
POST: @@ equilibrium 4 from the optimization.
POST: ba
... the command in full is BACK
POLY_3: ba
... the command in full is BACK

PARROT VERSION 5.3

Global minimization used as test only
PARROT: ed
... the command in full is EDIT_EXPERIMENTS
ED_EXP: read 1
... the command in full is READ_WORKSPACES
ED_EXP: s-we 0 4
... the command in full is SET_WEIGHT
ED_EXP: save
... the command in full is SAVE_WORKSPACES
ED_EXP: ba
... the command in full is BACK
PARROT: opt 0
... the command in full is OPTIMIZE_VARIABLES
Use      25 experiments, maximum is      2000
Use     494 real workspace, maximum is   50000
PARROT: l-r C SCREEN
... the command in full is LIST_RESULT

```

=====
OUTPUT FROM P A R R O T. DATE 2016. 5.16 14:20:24

\*\*\* SUCCESSFUL OPTIMIZATION. \*\*\*
NUMBER OF ITERATIONS: 0

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 0 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) \* 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.02757864E+04	2.02757864E+04	2.02757864E+04	7.39333291E-02
V2	-2.90134088E+01	-2.90134088E+01	-2.90134088E+01	3.44753302E-01
V11	-2.18127452E+04			
V12	1.55559572E+01			
V15	2.39869483E+04	2.39869483E+04	2.39869483E+04	6.19220768E-01
V16	-8.02178633E+00	-8.02178633E+00	-8.02178633E+00	2.18789658E+00
V17	3.13540526E+03	3.13540526E+03	3.13540526E+03	1.44882543E+00
V19	2.12643554E+04	2.12643554E+04	2.12643554E+04	4.78622311E+00
V20	-6.23643289E+00	-6.23643289E+00	-6.23643289E+00	1.26469088E+01

NUMBER OF OPTIMIZING VARIABLES : 7
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 3.83968704E-01 TO 7.37817472E+00
DEGREES OF FREEDOM 18. REDUCED SUM OF SQUARES 4.09898596E-01

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS
DX=2E-2, P0=101325, DH=500, DT=10

```

DEFINED FUNCTIONS AND VARIABLES%
HTR=HM(LIQUID)-HM(A2B)
1 T=1193 1187. 10.0 -5.532 -0.5532
1 W(LIQUID,B)=0.408 0.4157 2.00E-02 7.7215E-03 0.3861
1 W(BCC,B)=0.13 0.1332 2.00E-02 3.2119E-03 0.1606
2 T=1341 1317. 10.0 -24.32 -2.432
2 HTR=3727 3727. 5.00E+02 0.4611 9.2229E-04
3 T=1049 1047. 10.0 -1.990 -0.1990
3 W(LIQUID,A)=0.27 0.2739 2.00E-02 3.9062E-03 0.1953
3 W(BCC,A)=9.3E-2 9.4971E-02 2.00E-02 1.9713E-03 9.8563E-02
5 T=726 734.7 10.0 8.703 0.8703
5 X(BCC,B)=3.7E-2 3.9289E-02 2.00E-02 2.2886E-03 0.1144
5 X(BCC#2,A)=0.114 0.1200 2.00E-02 6.0001E-03 0.3000
6 X(BCC,B)=3.7E-2 3.6833E-02 2.00E-02 -1.6665E-04 -8.3327E-03
6 X(BCC#2,A)=0.114 0.1140 2.00E-02 -1.6829E-05 -8.4144E-04
10 W(LIQUID,A)=2E-2 1.9506E-02 2.00E-02 -4.9427E-04 -2.4713E-02
11 W(LIQUID,A)=4.2E-2 4.1827E-02 2.00E-02 -1.7330E-04 -8.6648E-03
12 W(LIQUID,A)=6.5E-2 6.5040E-02 2.00E-02 4.0133E-05 2.0066E-03
13 W(LIQUID,A)=9.3E-2 9.3114E-02 2.00E-02 1.1416E-04 5.7082E-03
20 W(LIQUID,A)=0.104 0.1043 2.00E-02 3.4980E-04 1.7490E-02
20 W(FCC,A)=3.8E-2 3.8244E-02 2.00E-02 2.4396E-04 1.2198E-02
21 W(LIQUID,A)=0.136 0.1375 2.00E-02 1.5284E-03 7.6418E-02
21 W(FCC,A)=4.7E-2 4.7395E-02 2.00E-02 3.9496E-04 1.9748E-02
22 W(LIQUID,A)=0.187 0.1886 2.00E-02 1.5692E-03 7.8460E-02
22 W(FCC,A)=5.9E-2 6.0019E-02 2.00E-02 1.0194E-03 5.0968E-02
23 W(LIQUID,A)=0.245 0.2474 2.00E-02 2.3699E-03 0.1185
23 W(BCC,A)=8.5E-2 8.6337E-02 2.00E-02 1.3367E-03 6.6834E-02

```

**PARROT:**  
**PARROT:Hit RETURN to continue**  
**PARROT:** opt 30

... the command in full is OPTIMIZE\_VARIABLES  
 Use 25 experiments, maximum is 2000  
 Use 494 real workspace, maximum is 50000  
 The following output is provided by subroutine VA05A

```

      AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 7.37817472E+00
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00

      AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 7.53019237E+00
1 1.0001E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00

      AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 7.11518144E+00
1 1.0000E+00 2 1.0001E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00

      AT THE 3 RD ITERATION WE HAVE THE SUM OF SQUARES 7.10968662E+00
1 1.0000E+00 2 1.0001E+00 3 1.0001E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00

      AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 7.11099046E+00
1 1.0000E+00 2 1.0001E+00 3 1.0001E+00 4 1.0001E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00

      AT THE 5 TH ITERATION WE HAVE THE SUM OF SQUARES 7.10983084E+00
1 1.0000E+00 2 1.0001E+00 3 1.0001E+00 4 1.0000E+00 5 1.0001E+00
6 1.0000E+00 7 1.0000E+00

      AT THE 6 TH ITERATION WE HAVE THE SUM OF SQUARES 7.10931183E+00
1 1.0000E+00 2 1.0001E+00 3 1.0001E+00 4 1.0000E+00 5 1.0000E+00
6 1.0001E+00 7 1.0000E+00

      AT THE 7 TH ITERATION WE HAVE THE SUM OF SQUARES 7.10944990E+00
1 1.0000E+00 2 1.0001E+00 3 1.0001E+00 4 1.0000E+00 5 1.0000E+00
6 1.0001E+00 7 1.0001E+00

      AT THE 8 TH ITERATION WE HAVE THE SUM OF SQUARES 3.63987301E-01
1 9.9778E-01 2 1.0040E+00 3 1.0002E+00 4 9.9998E-01 5 1.0000E+00
6 1.0001E+00 7 1.0000E+00

      AT THE 9 TH ITERATION WE HAVE THE SUM OF SQUARES 3.27827938E-01
1 9.9774E-01 2 1.0037E+00 3 1.0002E+00 4 9.9757E-01 5 9.9826E-01
6 1.0015E+00 7 1.0030E+00

      AT THE 10 TH ITERATION WE HAVE THE SUM OF SQUARES 2.68447716E-01
1 9.9735E-01 2 1.0038E+00 3 9.9865E-01 4 9.9067E-01 5 9.9310E-01
6 1.0027E+00 7 1.0046E+00

      AT THE 11 TH ITERATION WE HAVE THE SUM OF SQUARES 2.16955159E-01
1 9.9691E-01 2 1.0034E+00 3 9.9639E-01 4 9.8058E-01 5 9.8548E-01
6 1.0080E+00 7 1.0160E+00

      AT THE 12 TH ITERATION WE HAVE THE SUM OF SQUARES 1.51367607E-01
1 9.9564E-01 2 1.0029E+00 3 9.8912E-01 4 9.5293E-01 5 9.6407E-01
6 1.0089E+00 7 1.0123E+00

      THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 12 iterations
1 9.9564E-01 2 1.0029E+00 3 9.8912E-01 4 9.5293E-01 5 9.6407E-01
6 1.0089E+00 7 1.0123E+00

1 7.0458E-02 2 -3.9714E-02 3 -7.7917E-02 4 -7.3557E-02 5 5.9818E-02
6 2.5625E-01 7 -1.8711E-02 8 -9.5448E-02 9 1.6592E-01 10 5.4874E-02
11 -3.7948E-02 12 3.1686E-02 13 -9.3446E-02 14 -2.8663E-02 15 -1.6943E-02
16 -1.0570E-02 17 -1.1807E-02 18 -1.9285E-03 19 -9.4044E-03 20 5.1591E-02
21 -1.0495E-02 22 4.5740E-02 23 2.4209E-03 24 1.2336E-02 25 -8.0309E-02

```

THE SUM OF SQUARES IS 1.51367607E-01

**PARROT:** cont 30  
 ... the command in full is CONTINUE\_OPTIMIZATION

It is safe to CONTINUE only after TOO MANY ITERATIONS  
 and no change in variables and experiments ...  
 Now anything can happen ...

**PARROT:** l-r C SCREEN  
 ... the command in full is LIST\_RESULT

=====  
 OUTPUT FROM P A R R O T. DATE 2016. 5.16 14:20:24



\*\*\* SUCCESSFUL OPTIMIZATION. \*\*\*  
NUMBER OF ITERATIONS: 13

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N  
MINIMUM SAVE ON FILE: Y  
ERROR FOR INEQUALITIES = 1.00000000E+00  
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04  
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)  
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04  
ACC = (INITIAL SUM OF SQUARES) \* 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.01874435E+04	2.02757864E+04	2.02757864E+04	2.69317159E-02
V2	-2.90969417E+01	-2.90134088E+01	-2.90134088E+01	1.50772675E-02
V11	-2.18127452E+04			
V12	1.55559572E+01			
V15	2.37258616E+04	2.39869483E+04	2.39869483E+04	9.90009036E-02
V16	-7.64416251E+00	-8.02178633E+00	-8.02178633E+00	3.01534612E-01
V17	3.02274705E+03	3.13540526E+03	3.13540526E+03	2.49736435E-01
V19	2.14533478E+04	2.12643554E+04	2.12643554E+04	6.60453317E-01
V20	-6.31327793E+00	-6.23643289E+00	-6.23643289E+00	1.71543397E+00

NUMBER OF OPTIMIZING VARIABLES : 7  
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO  
THE SUM OF SQUARES HAS CHANGED FROM 7.37817472E+00 TO 1.51367607E-01  
DEGREES OF FREEDOM 18. REDUCED SUM OF SQUARES 8.40931149E-03

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS

DX=2E-2, P0=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%

HTR=HM(LIQUID)-HM(A2B)

1 T=1193	1194.	10.0	0.7046	7.0458E-02
1 W(LIQUID,B)=0.408	0.4072	2.00E-02	-7.9429E-04	-3.9714E-02
1 W(BCC,B)=0.13	0.1284	2.00E-02	-1.5583E-03	-7.7917E-02
2 T=1341	1340.	10.0	-0.7356	-7.3557E-02
2 HTR=3727	3757.	5.00E+02	29.91	5.9818E-02
3 T=1049	1052.	10.0	2.563	0.2563
3 W(LIQUID,A)=0.27	0.2696	2.00E-02	-3.7422E-04	-1.8711E-02
3 W(BCC,A)=9.3E-2	9.1091E-02	2.00E-02	-1.9090E-03	-9.5448E-02
5 T=726	727.7	10.0	1.659	0.1659
5 X(BCC,B)=3.7E-2	3.8097E-02	2.00E-02	1.0975E-03	5.4874E-02
5 X(BCC#2,A)=0.114	0.1132	2.00E-02	-7.5897E-04	-3.7948E-02
6 X(BCC,B)=3.7E-2	3.7634E-02	2.00E-02	6.3372E-04	3.1686E-02
6 X(BCC#2,A)=0.114	0.1121	2.00E-02	-1.8689E-03	-9.3446E-02
10 W(LIQUID,A)=2E-2	1.9427E-02	2.00E-02	-5.7326E-04	-2.8663E-02
11 W(LIQUID,A)=4.2E-2	4.1661E-02	2.00E-02	-3.3885E-04	-1.6943E-02
12 W(LIQUID,A)=6.5E-2	6.4789E-02	2.00E-02	-2.1139E-04	-1.0570E-02
13 W(LIQUID,A)=9.3E-2	9.2764E-02	2.00E-02	-2.3614E-04	-1.1807E-02
20 W(LIQUID,A)=0.104	0.1040	2.00E-02	-3.8571E-05	-1.9285E-03
20 W(FCC,A)=3.8E-2	3.7812E-02	2.00E-02	-1.8809E-04	-9.4044E-03
21 W(LIQUID,A)=0.136	0.1370	2.00E-02	1.0318E-03	5.1591E-02
21 W(FCC,A)=4.7E-2	4.6790E-02	2.00E-02	-2.0989E-04	-1.0495E-02
22 W(LIQUID,A)=0.187	0.1879	2.00E-02	9.1479E-04	4.5740E-02
22 W(FCC,A)=5.9E-2	5.9048E-02	2.00E-02	4.8418E-05	2.4209E-03
23 W(LIQUID,A)=0.245	0.2452	2.00E-02	2.4672E-04	1.2336E-02
23 W(BCC,A)=8.5E-2	8.3394E-02	2.00E-02	-1.6062E-03	-8.0309E-02

PARROT:

PARROT:Hit RETURN to continue

PARROT: @@ Optimization converged, try to add equilibrium 4 again

PARROT: ed

... the command in full is EDIT\_EXPERIMENTS

ED\_EXP: read 1

... the command in full is READ\_WORKSPACES

ED\_EXP: s-e 4

... the command in full is SELECT\_EQUILIBRIUM

Equilibrium number 4, label AINV

ED\_EXP: s-a-s

... the command in full is SET\_ALL\_START\_VALUES

T /1204.671469/: 1200

Automatic start values for phase constituents? /N/: N

Phase LIQUID

Major constituent(s) /b/: b

Phase BCC

Major constituent(s) /b/: b

Phase FCC

Major constituent(s) /b/: b

ED\_EXP:

ED\_EXP: c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Testing result with global minimization

14 ITS, CPU TIME USED 0 SECONDS

ED\_EXP: l-e

... the command in full is LIST\_EQUILIBRIUM

OUTPUT TO SCREEN OR FILE /SCREEN/:

Options /VWCS/: VWCS

Output from POLY-3, equilibrium = 4, label AINV, database:

Conditions:

P=1.01325E5

FIXED PHASES

LIQUID=1 BCC=1 FCC=1

DEGREES OF FREEDOM 0

Temperature 1194.80 K ( 921.65 C), Pressure 1.013250E+05

Number of moles of components 3.00000E+00, Mass in grams 1.29837E+02  
Total Gibbs energy -9.46749E+03, Enthalpy 1.96784E+04, Volume 0.00000E+00

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
A	6.7209E-01	1.0353E-01	4.0897E-01	-8.8824E+03	SER
B	2.3279E+00	8.9647E-01	8.5964E-01	-1.5025E+03	SER

FCC Status FIXED Driving force 0.0000E+00  
Moles 1.0000E+00, Mass 4.5830E+01, Volume fraction 0.0000E+00 Mass fractions:  
B 9.39335E-01 A 6.06655E-02

BCC Status FIXED Driving force 0.0000E+00  
Moles 1.0000E+00, Mass 4.5327E+01, Volume fraction 0.0000E+00 Mass fractions:  
B 9.31263E-01 A 6.87372E-02

LIQUID Status FIXED Driving force 0.0000E+00  
Moles 1.0000E+00, Mass 3.8681E+01, Volume fraction 0.0000E+00 Mass fractions:  
B 8.04923E-01 A 1.95077E-01

SET WEIGHT 0,,,  
EXPERIMENT T=1203:DT  
EXPERIMENT W(LIQUID,A)=0.19:DX  
EXPERIMENT W(BCC,A)=6.9E-2:DX  
EXPERIMENT W(FCC,A)=6E-2:DX

ED\_EXP: ba

... the command in full is BACK

PARROT: @@ It still fails, try to calculate the phase diagram again.

PARROT: mac tcex36cpd

... the command in full is MACRO\_FILE\_OPEN

PARROT: set-echo

NO SUCH COMMAND, USE HELP

PARROT: @@ Calculate the phase diagram

PARROT: @@ This TCM should be run in PARROT

PARROT: go p-3

... the command in full is GOTO\_MODULE

POLY\_3:

POLY\_3: @@ In PARROT, the global minimization is turned off automatically.

POLY\_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning

POLY\_3: @@ message will be given.

POLY\_3:

POLY\_3: advanced-option global yes,,

... the command in full is ADVANCED\_OPTIONS

Settings for global minimization:

\*\*\* WARNING \*\*\* Global equilibrium calculation may create new composition sets  
and this may corrupt your PARROT work file (.PAR file).

Do not go back to PARROT but exit from POLY after your POLY calculations.

POLY\_3:

POLY\_3: def-com,,,,

... the command in full is DEFINE\_COMPONENTS

POLY\_3: s-a-v 1 w(b) 0 1,,,,

... the command in full is SET\_AXIS\_VARIABLE

The condition W(B)=.1234 created

POLY\_3: s-a-v 2 t 300 1700,,,,

... the command in full is SET\_AXIS\_VARIABLE

The condition T=942.2 created

POLY\_3: s-c t=500

... the command in full is SET\_CONDITION

POLY\_3: l-c

... the command in full is LIST\_CONDITIONS

W(B)=0.1234, P=1E5, N=1, T=500

DEGREES OF FREEDOM 0

POLY\_3: c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Using global minimization procedure

Calculated 412 grid points in 0 s

Found the set of lowest grid points in 0 s

Calculated POLY solution 0 s, total time 0 s

POLY\_3: save tcex36 y

... the command in full is SAVE\_WORKSPACES

This file contains results from a previous STEP or MAP command.

The SAVE command will save the current status of the program but destroy  
the results from the previous STEP or MAP commands.

POLY\_3: map

Version 3 mapping is selected

Generating start equilibrium 1

Generating start equilibrium 2

Generating start equilibrium 3

Generating start equilibrium 4

Generating start equilibrium 5

Generating start equilibrium 6

Generating start equilibrium 7

Generating start equilibrium 8

Generating start equilibrium 9

Generating start equilibrium 10

Generating start equilibrium 11

Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1

Generating start point 2

Generating start point 3

Generating start point 4

Generating start point 5

Generating start point 6

Generating start point 7

Generating start point 8

Generating start point 9

Generating start point 10

Working hard

Generating start point 11

Generating start point 12

Generating start point 13

Generating start point 14

Generating start point 15

Generating start point 16

Generating start point 17

Generating start point 18

Generating start point 19

Generating start point 20

Working hard

```

Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

Phase region boundary 1 at: 7.140E-01 3.100E+02
  BCC
  ** BCC#2
Calculated.. 2 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 7.141E-01 3.000E+02
  BCC
  ** BCC#2
Calculated. 14 equilibria

Phase region boundary 3 at: 6.826E-01 7.277E+02
  ** A2B
  BCC
  ** BCC#2

Phase region boundary 4 at: 3.631E-01 7.277E+02
  ** A2B
  BCC
Calculated. 15 equilibria

Phase region boundary 5 at: 3.764E-01 1.194E+03
  ** LIQUID
  ** A2B
  BCC

Phase region boundary 6 at: 2.817E-01 1.194E+03
  ** LIQUID
  BCC
Calculated 24 equilibria

Phase region boundary 7 at: 4.860E-01 1.194E+03
  ** LIQUID
  A2B
Calculated. 28 equilibria

Phase region boundary 8 at: 6.504E-01 1.052E+03
  ** LIQUID
  A2B
  ** BCC

Phase region boundary 9 at: 7.656E-01 1.052E+03
  A2B
  ** BCC
Calculated. 11 equilibria
Terminating at known equilibrium

Phase region boundary 10 at: 8.290E-01 1.052E+03
  LIQUID
  ** BCC
Calculated. 8 equilibria

Phase region boundary 11 at: 8.731E-01 1.195E+03
  LIQUID
  ** BCC
  ** FCC

Phase region boundary 12 at: 8.778E-01 1.195E+03
  LIQUID
  ** FCC
Calculated 36 equilibria

Phase region boundary 13 at: 9.353E-01 1.195E+03
  BCC
  ** FCC
Calculated 21 equilibria

Phase region boundary 14 at: 7.140E-01 3.100E+02
  BCC
  ** BCC#2
Calculated. 13 equilibria
Terminating at known equilibrium

Phase region boundary 15 at: 7.140E-01 3.100E+02
  BCC
  ** BCC#2
Calculated.. 2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 16 at: 7.140E-01 3.100E+02
  BCC
  ** BCC#2
Calculated. 13 equilibria
Terminating at known equilibrium

Phase region boundary 17 at: 7.140E-01 3.100E+02
  BCC
  ** BCC#2
Calculated.. 2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 18 at: 7.140E-01 3.100E+02
  BCC
  ** BCC#2
Calculated. 13 equilibria
Terminating at known equilibrium

Phase region boundary 19 at: 7.140E-01 3.100E+02
  BCC
  ** BCC#2
Calculated.. 2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 20 at: 7.140E-01 3.100E+02

```

```

      BCC
** BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 21 at:  7.140E-01  3.100E+02
** BCC
   BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 22 at:  7.140E-01  3.100E+02
** BCC
   BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 23 at:  7.140E-01  3.100E+02
** BCC
   BCC#2
Calculated..         2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 24 at:  7.140E-01  3.100E+02
** BCC
   BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 25 at:  3.649E-01  7.700E+02
** A2B
   BCC
Calculated           10 equilibria

Phase region boundary 26 at:  3.649E-01  7.700E+02
** A2B
   BCC
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 27 at:  3.649E-01  7.700E+02
** A2B
   BCC
Calculated.          14 equilibria
Terminating at known equilibrium

Phase region boundary 28 at:  7.918E-01  7.700E+02
** A2B
   BCC
Calculated           10 equilibria

Phase region boundary 29 at:  7.918E-01  7.700E+02
** A2B
   BCC
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 30 at:  7.918E-01  7.700E+02
** A2B
   BCC
Calculated.          10 equilibria
Terminating at known equilibrium

Phase region boundary 31 at:  2.447E-01  1.230E+03
** LIQUID
   BCC
Calculated.          4 equilibria
Terminating at known equilibrium

Phase region boundary 32 at:  2.447E-01  1.230E+03
** LIQUID
   BCC
Calculated           26 equilibria

Phase region boundary 33 at:  8.855E-01  1.230E+03
** LIQUID
   FCC
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 34 at:  8.855E-01  1.230E+03
** LIQUID
   FCC
Calculated           29 equilibria

Phase region boundary 35 at:  6.403E-03  1.397E+03
   LIQUID
** BCC
Calculated           9 equilibria

Phase region boundary 36 at:  6.403E-03  1.397E+03
   LIQUID
** BCC
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 37 at:  2.294E-01  1.244E+03
   LIQUID
** BCC
Calculated           21 equilibria

Phase region boundary 38 at:  2.294E-01  1.244E+03
   LIQUID
** BCC
Calculated.          4 equilibria
Terminating at known equilibrium

Phase region boundary 39 at:  6.122E-01  1.242E+03
   LIQUID
** A2B
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 40 at:  6.122E-01  1.242E+03

```

```

    LIQUID
** A2B
Calculated.          8  equilibria
Terminating at known equilibrium

Phase region boundary 41 at:  9.927E-01  1.613E+03
    LIQUID
** FCC
Calculated.          20  equilibria
Terminating at known equilibrium

Phase region boundary 42 at:  9.927E-01  1.613E+03
    LIQUID
** FCC
Calculated          13  equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tce
x36.POLY3
CPU time for mapping          1  seconds
POLY_3: post

```

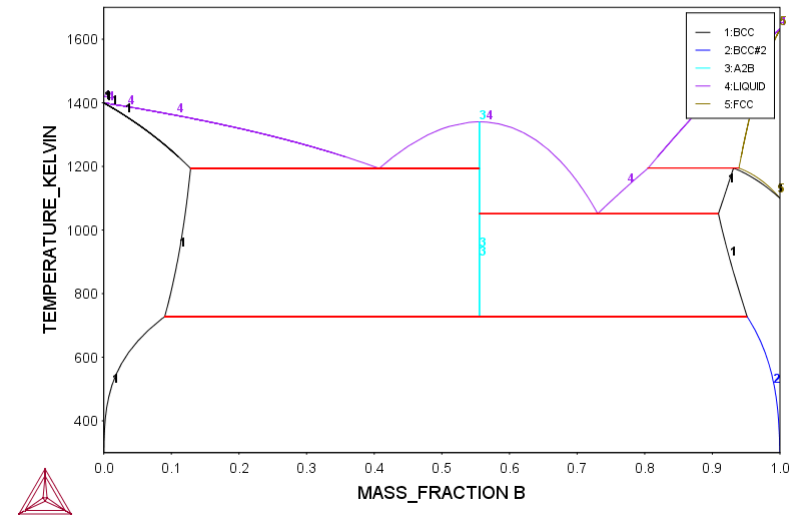
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

```

POST: s-l d
... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
... the command in full is PLOT DIAGRAM
2016.05.16.14.20.28
A,B
P=1E5,N=1

```



```

POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:Hit RETURN to continue
POST: @@ Sometimes a very strange shape of the fcc phase here and no
POST: @@ equilibrium between liq, fcc and bcc at high B content.
POST: ba
... the command in full is BACK
POLY_3: ba
... the command in full is BACK

```

PARROT VERSION 5.3

```

Global minimization used as test only
PARROT: l-r C SCREEN
... the command in full is LIST_RESULT

```

```

=====
OUTPUT FROM P A R R O T.  DATE 2016. 5.16  14:20:28

```

```

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 13

```

== OPTIMIZING CONDITIONS ==

```

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 30  DMAX = 1.00000000E+02  H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

```

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

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V11	-2.18127452E+04			
V12	1.55559572E+01			
V15	2.37258616E+04	2.39869483E+04	2.39869483E+04	9.90009036E-02
V16	-7.64416251E+00	-8.02178633E+00	-8.02178633E+00	3.01534612E-01

```
V17      3.02274705E+03      3.13540526E+03      3.13540526E+03      2.49736435E-01
V19      2.14533478E+04      2.12643554E+04      2.12643554E+04      6.60453317E-01
V20     -6.31327793E+00     -6.23643289E+00     -6.23643289E+00      1.71543397E+00
```

NUMBER OF OPTIMIZING VARIABLES : 7  
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO  
THE SUM OF SQUARES HAS CHANGED FROM 7.37817472E+00 TO 1.51367607E-01  
DEGREES OF FREEDOM 18. REDUCED SUM OF SQUARES 8.40931149E-03

\$ ===== BLOCK NUMBER 1

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```
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1 W(BCC,B)=0.13      0.1284      2.00E-02      -1.5583E-03      -7.7917E-02
2 T=1341      1340.      10.0      -0.7356      -7.3557E-02
2 HTR=3727      3757.      5.00E+02      29.91      5.9818E-02
3 T=1049      1052.      10.0      2.563      0.2563
3 W(LIQUID,A)=0.27      0.2696      2.00E-02      -3.7422E-04      -1.8711E-02
3 W(BCC,A)=9.3E-2      9.1091E-02      2.00E-02      -1.9090E-03      -9.5448E-02
5 T=726      727.7      10.0      1.659      0.1659
5 X(BCC,B)=3.7E-2      3.8097E-02      2.00E-02      1.0975E-03      5.4874E-02
5 X(BCC#2,A)=0.114      0.1132      2.00E-02      -7.5897E-04      -3.7948E-02
6 X(BCC,B)=3.7E-2      3.7634E-02      2.00E-02      6.3372E-04      3.1686E-02
6 X(BCC#2,A)=0.114      0.1121      2.00E-02      -1.8689E-03      -9.3446E-02
10 W(LIQUID,A)=2E-2      1.9427E-02      2.00E-02      -5.7326E-04      -2.8663E-02
11 W(LIQUID,A)=4.2E-2      4.1661E-02      2.00E-02      -3.3885E-04      -1.6943E-02
12 W(LIQUID,A)=6.5E-2      6.4789E-02      2.00E-02      -2.1139E-04      -1.0570E-02
13 W(LIQUID,A)=9.3E-2      9.2764E-02      2.00E-02      -2.3614E-04      -1.1807E-02
20 W(LIQUID,A)=0.104      0.1040      2.00E-02      -3.8571E-05      -1.9285E-03
20 W(FCC,A)=3.8E-2      3.7812E-02      2.00E-02      -1.8809E-04      -9.4044E-03
21 W(LIQUID,A)=0.136      0.1370      2.00E-02      1.0318E-03      5.1591E-02
21 W(FCC,A)=4.7E-2      4.6790E-02      2.00E-02      -2.0989E-04      -1.0495E-02
22 W(LIQUID,A)=0.187      0.1879      2.00E-02      9.1479E-04      4.5740E-02
22 W(FCC,A)=5.9E-2      5.9048E-02      2.00E-02      4.8418E-05      2.4209E-03
23 W(LIQUID,A)=0.245      0.2452      2.00E-02      2.4672E-04      1.2336E-02
23 W(BCC,A)=8.5E-2      8.3394E-02      2.00E-02      -1.6062E-03      -8.0309E-02
```

PARROT:

PARROT: @@ Note that all other experiments are well fitted!

PARROT: @@ Try to improve by optimizing a little more !!!

PARROT: resc

... the command in full is RESCALE\_VARIABLES

PARROT: opt 30

... the command in full is OPTIMIZE\_VARIABLES

Use 25 experiments, maximum is 2000

Use 494 real workspace, maximum is 50000

The following output is provided by subroutine VA05A

```
AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 1.51367607E-01
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00
```

```
AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 1.52533051E-01
1 1.0001E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00
```

```
AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 1.53440354E-01
1 1.0000E+00 2 1.0001E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00
```

```
AT THE 3 RD ITERATION WE HAVE THE SUM OF SQUARES 1.50571317E-01
1 1.0000E+00 2 1.0000E+00 3 1.0001E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00
```

```
AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 1.50814099E-01
1 1.0000E+00 2 1.0000E+00 3 1.0001E+00 4 1.0001E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00
```

```
AT THE 5 TH ITERATION WE HAVE THE SUM OF SQUARES 1.50610770E-01
1 1.0000E+00 2 1.0000E+00 3 1.0001E+00 4 1.0000E+00 5 1.0001E+00
6 1.0000E+00 7 1.0000E+00
```

```
AT THE 6 TH ITERATION WE HAVE THE SUM OF SQUARES 1.50503265E-01
1 1.0000E+00 2 1.0000E+00 3 1.0001E+00 4 1.0000E+00 5 1.0000E+00
6 1.0001E+00 7 1.0000E+00
```

```
AT THE 7 TH ITERATION WE HAVE THE SUM OF SQUARES 1.50524533E-01
1 1.0000E+00 2 1.0000E+00 3 1.0001E+00 4 1.0000E+00 5 1.0000E+00
6 1.0001E+00 7 1.0001E+00
```

```
AT THE 8 TH ITERATION WE HAVE THE SUM OF SQUARES 1.50302078E-01
1 9.9999E-01 2 1.0000E+00 3 1.0001E+00 4 9.9998E-01 5 9.9999E-01
6 1.0001E+00 7 1.0001E+00
```

```
AT THE 9 TH ITERATION WE HAVE THE SUM OF SQUARES 1.50110907E-01
1 1.0000E+00 2 1.0000E+00 3 1.0001E+00 4 9.9996E-01 5 9.9998E-01
6 1.0002E+00 7 1.0002E+00
```

```
AT THE 10 TH ITERATION WE HAVE THE SUM OF SQUARES 1.49917194E-01
1 9.9999E-01 2 1.0000E+00 3 1.0002E+00 4 9.9992E-01 5 9.9996E-01
6 1.0002E+00 7 1.0003E+00
```

```
AT THE 11 TH ITERATION WE HAVE THE SUM OF SQUARES 1.49701897E-01
1 9.9999E-01 2 1.0000E+00 3 1.0002E+00 4 9.9986E-01 5 9.9992E-01
6 1.0004E+00 7 1.0007E+00
```

```
AT THE 12 TH ITERATION WE HAVE THE SUM OF SQUARES 1.49443230E-01
1 9.9998E-01 2 1.0000E+00 3 1.0002E+00 4 9.9974E-01 5 9.9985E-01
6 1.0007E+00 7 1.0014E+00
```

```
AT THE 13 TH ITERATION WE HAVE THE SUM OF SQUARES 1.49088139E-01
1 9.9998E-01 2 1.0000E+00 3 1.0001E+00 4 9.9950E-01 5 9.9971E-01
6 1.0013E+00 7 1.0029E+00
```

```
AT THE 14 TH ITERATION WE HAVE THE SUM OF SQUARES 1.48551477E-01
1 9.9996E-01 2 1.0000E+00 3 1.0000E+00 4 9.9904E-01 5 9.9942E-01
6 1.0024E+00 7 1.0058E+00
```

```

      AT THE 15 TH ITERATION WE HAVE THE SUM OF SQUARES 1.49192907E-01
1 1.0001E+00 2 1.0000E+00 3 1.0000E+00 4 9.9904E-01 5 9.9942E-01
6 1.0025E+00 7 1.0058E+00

      AT THE 16 TH ITERATION WE HAVE THE SUM OF SQUARES 1.50825500E-01
1 9.9998E-01 2 1.0001E+00 3 1.0000E+00 4 9.9903E-01 5 9.9942E-01
6 1.0024E+00 7 1.0058E+00

      AT THE 17 TH ITERATION WE HAVE THE SUM OF SQUARES 1.48149051E-01
1 9.9998E-01 2 9.9998E-01 3 1.0001E+00 4 9.9903E-01 5 9.9942E-01
6 1.0024E+00 7 1.0058E+00

      AT THE 18 TH ITERATION WE HAVE THE SUM OF SQUARES 1.48106327E-01
1 9.9997E-01 2 1.0000E+00 3 1.0001E+00 4 9.9912E-01 5 9.9942E-01
6 1.0024E+00 7 1.0059E+00

      AT THE 19 TH ITERATION WE HAVE THE SUM OF SQUARES 1.48103802E-01
1 9.9996E-01 2 1.0000E+00 3 1.0001E+00 4 9.9912E-01 5 9.9951E-01
6 1.0025E+00 7 1.0059E+00

      AT THE 20 TH ITERATION WE HAVE THE SUM OF SQUARES 1.47348969E-01
1 9.9995E-01 2 9.9998E-01 3 9.9990E-01 4 9.9819E-01 5 9.9893E-01
6 1.0048E+00 7 1.0117E+00

      AT THE 21 TH ITERATION WE HAVE THE SUM OF SQUARES 1.48042770E-01
1 9.9997E-01 2 9.9996E-01 3 9.9986E-01 4 9.9823E-01 5 9.9895E-01
6 1.0047E+00 7 1.0117E+00

      AT THE 22 TH ITERATION WE HAVE THE SUM OF SQUARES 1.46175461E-01
1 9.9990E-01 2 9.9997E-01 3 9.9943E-01 4 9.9635E-01 5 9.9778E-01
6 1.0094E+00 7 1.0234E+00

      AT THE 23 TH ITERATION WE HAVE THE SUM OF SQUARES 1.44759679E-01
1 9.9981E-01 2 9.9992E-01 3 9.9844E-01 4 9.9265E-01 5 9.9546E-01
6 1.0188E+00 7 1.0468E+00

      AT THE 24 TH ITERATION WE HAVE THE SUM OF SQUARES 1.44427075E-01
1 9.9973E-01 2 9.9989E-01 3 9.9765E-01 4 9.8970E-01 5 9.9361E-01
6 1.0261E+00 7 1.0652E+00

      THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 24 iterations
1 9.9973E-01 2 9.9989E-01 3 9.9765E-01 4 9.8970E-01 5 9.9361E-01
6 1.0261E+00 7 1.0652E+00

1 6.6807E-02 2 -4.4958E-02 3 -9.7560E-02 4 -6.3010E-02 5 6.3385E-02
6 2.1373E-01 7 -2.7115E-02 8 -1.2155E-01 9 1.5013E-01 10 5.9941E-02
11 -5.8436E-02 12 3.8935E-02 13 -1.0845E-01 14 -2.2928E-02 15 -7.7951E-03
16 -8.4310E-04 17 -4.6848E-03 18 3.2982E-03 19 -3.5905E-03 20 4.8873E-02
21 -1.3805E-02 22 2.5374E-02 23 -2.7745E-02 24 -7.5343E-03 25 -1.0836E-01

```

THE SUM OF SQUARES IS 1.44427075E-01

PARROT: l-r C SCREEN

... the command in full is LIST\_RESULT

```

=====
OUTPUT FROM P A R R O T. DATE 2016. 5.16 14:20:28

```

\*\*\* SUCCESSFUL OPTIMIZATION. \*\*\*  
NUMBER OF ITERATIONS: 25

== OPTIMIZING CONDITIONS ==

```

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

```

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.01820918E+04	2.01874435E+04	2.01874435E+04	2.60519708E-02
V2	-2.90936108E+01	-2.90969417E+01	-2.90969417E+01	1.41576502E-02
V11	-2.18127452E+04			
V12	1.55559572E+01			
V15	2.36701045E+04	2.37258616E+04	2.37258616E+04	1.00528943E-01
V16	-7.56540324E+00	-7.64416251E+00	-7.64416251E+00	3.17219075E-01
V17	3.00342248E+03	3.02274705E+03	3.02274705E+03	2.60675642E-01
V19	2.20133196E+04	2.14533478E+04	2.14533478E+04	6.92926768E-01
V20	-6.72497818E+00	-6.31327793E+00	-6.31327793E+00	1.79244330E+00

NUMBER OF OPTIMIZING VARIABLES : 7  
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO  
THE SUM OF SQUARES HAS CHANGED FROM 1.51367607E-01 TO 1.44427075E-01  
DEGREES OF FREEDOM 18. REDUCED SUM OF SQUARES 8.02372640E-03

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS

DX=2E-2, P0=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%

HTR=HM(LIQUID)-HM(A2B)

1 T=1193	1194.	10.0	0.6681	6.6807E-02
1 W(LIQUID,B)=0.408	0.4071	2.00E-02	-8.9916E-04	-4.4958E-02
1 W(BCC,B)=0.13	0.1280	2.00E-02	-1.9512E-03	-9.7560E-02
2 T=1341	1340.	10.0	-0.6301	-6.3010E-02
2 HTR=3727	3759.	5.00E+02	31.69	6.3385E-02
3 T=1049	1051.	10.0	2.137	0.2137
3 W(LIQUID,A)=0.27	0.2695	2.00E-02	-5.4230E-04	-2.7115E-02
3 W(BCC,A)=9.3E-2	9.0569E-02	2.00E-02	-2.4311E-03	-0.1216
5 T=726	727.5	10.0	1.501	0.1501
5 X(BCC,B)=3.7E-2	3.8199E-02	2.00E-02	1.1988E-03	5.9941E-02

5	X(BCC#2,A)=0.114	0.1128	2.00E-02	-1.1687E-03	-5.8436E-02
6	X(BCC,B)=3.7E-2	3.7779E-02	2.00E-02	7.7870E-04	3.8935E-02
6	X(BCC#2,A)=0.114	0.1118	2.00E-02	-2.1691E-03	-0.1085
10	W(LIQUID,A)=2E-2	1.9541E-02	2.00E-02	-4.5856E-04	-2.2928E-02
11	W(LIQUID,A)=4.2E-2	4.1844E-02	2.00E-02	-1.5590E-04	-7.7951E-03
12	W(LIQUID,A)=6.5E-2	6.4983E-02	2.00E-02	-1.6862E-05	-8.4310E-04
13	W(LIQUID,A)=9.3E-2	9.2906E-02	2.00E-02	-9.3697E-05	-4.6848E-03
20	W(LIQUID,A)=0.104	0.1041	2.00E-02	6.5965E-05	3.2982E-03
20	W(FCC,A)=3.8E-2	3.7928E-02	2.00E-02	-7.1810E-05	-3.5905E-03
21	W(LIQUID,A)=0.136	0.1370	2.00E-02	9.7746E-04	4.8873E-02
21	W(FCC,A)=4.7E-2	4.6724E-02	2.00E-02	-2.7609E-04	-1.3805E-02
22	W(LIQUID,A)=0.187	0.1875	2.00E-02	5.0747E-04	2.5374E-02
22	W(FCC,A)=5.9E-2	5.8445E-02	2.00E-02	-5.5491E-04	-2.7745E-02
23	W(LIQUID,A)=0.245	0.2448	2.00E-02	-1.5069E-04	-7.5343E-03
23	W(BCC,A)=8.5E-2	8.2833E-02	2.00E-02	-2.1672E-03	-0.1084

```

PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ Calculate the phase diagram again
PARROT: mac tcex36cpd
... the command in full is MACRO_FILE_OPEN
PARROT: set-echo
NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
... the command in full is GOTO_MODULE
POLY_3:
POLY_3: @@ In PARROT, the global minimization is turned off automatically.
POLY_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY_3: @@ message will be given.
POLY_3:
POLY_3: advanced-option global yes,,
... the command in full is ADVANCED_OPTIONS
Settings for global minimization:
*** WARNING *** Global equilibrium calculation may create new composition sets
and this may corrupt your PARROT work file (.PAR file).
Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY_3:
POLY_3: def-com,,,,
... the command in full is DEFINE_COMPONENTS
POLY_3: s-a-v 1 w(b) 0 1,,,,
... the command in full is SET_AXIS_VARIABLE
The condition W(B)=.1234 created
POLY_3: s-a-v 2 t 300 1700,,,,
... the command in full is SET_AXIS_VARIABLE
The condition T=942.2 created
POLY_3: s-c t=500
... the command in full is SET_CONDITION
POLY_3: l-c
... the command in full is LIST_CONDITIONS
W(B)=0.1234, P=1E5, N=1, T=500
DEGREES OF FREEDOM 0
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 412 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY_3: save tcex36 y
... the command in full is SAVE_WORKSPACES

```

This file contains results from a previous STEP or MAP command.  
The SAVE command will save the current status of the program but destroy  
the results from the previous STEP or MAP commands.

```

POLY_3: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

```

Organizing start points

Using ADDED start equilibria

```

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27

```



```

Generating start point 28

Phase region boundary 1 at: 7.140E-01 3.100E+02
  BCC
  ** BCC#2
Calculated.. 2 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 7.141E-01 3.000E+02
  BCC
  ** BCC#2
Calculated. 14 equilibria

Phase region boundary 3 at: 6.828E-01 7.275E+02
  ** A2B
  BCC
  ** BCC#2

Phase region boundary 4 at: 3.632E-01 7.275E+02
  ** A2B
  BCC
Calculated. 15 equilibria

Phase region boundary 5 at: 3.763E-01 1.194E+03
  ** LIQUID
  ** A2B
  BCC

Phase region boundary 6 at: 2.815E-01 1.194E+03
  ** LIQUID
  BCC
Calculated 27 equilibria

Phase region boundary 7 at: 4.860E-01 1.194E+03
  ** LIQUID
  A2B
Calculated. 28 equilibria

Phase region boundary 8 at: 6.505E-01 1.051E+03
  ** LIQUID
  A2B
  ** BCC

Phase region boundary 9 at: 7.660E-01 1.051E+03
  A2B
  ** BCC
Calculated. 11 equilibria
Terminating at known equilibrium

Phase region boundary 10 at: 8.294E-01 1.051E+03
  LIQUID
  ** BCC
Calculated. 8 equilibria

Phase region boundary 11 at: 8.737E-01 1.195E+03
  LIQUID
  ** BCC
  ** FCC

Phase region boundary 12 at: 8.785E-01 1.195E+03
  LIQUID
  ** FCC
Calculated 31 equilibria

Phase region boundary 13 at: 9.360E-01 1.195E+03
  BCC
  ** FCC
Calculated 27 equilibria

Phase region boundary 14 at: 7.140E-01 3.100E+02
  BCC
  ** BCC#2
Calculated. 13 equilibria
Terminating at known equilibrium

Phase region boundary 15 at: 7.140E-01 3.100E+02
  BCC
  ** BCC#2
Calculated.. 2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 16 at: 7.140E-01 3.100E+02
  BCC
  ** BCC#2
Calculated. 13 equilibria
Terminating at known equilibrium

Phase region boundary 17 at: 7.140E-01 3.100E+02
  BCC
  ** BCC#2
Calculated.. 2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 18 at: 7.140E-01 3.100E+02
  BCC
  ** BCC#2
Calculated. 13 equilibria
Terminating at known equilibrium

Phase region boundary 19 at: 7.140E-01 3.100E+02
  BCC
  ** BCC#2
Calculated.. 2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 20 at: 7.140E-01 3.100E+02
  BCC
  ** BCC#2
Calculated. 13 equilibria
Terminating at known equilibrium

Phase region boundary 21 at: 7.140E-01 3.100E+02
  ** BCC

```

BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 22 at: 7.140E-01 3.100E+02  
 \*\* BCC  
 BCC#2  
 Calculated.. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 23 at: 7.140E-01 3.100E+02  
 \*\* BCC  
 BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 24 at: 7.140E-01 3.100E+02  
 \*\* BCC  
 BCC#2  
 Calculated.. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 25 at: 3.650E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated 10 equilibria

Phase region boundary 26 at: 3.650E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated.. 3 equilibria  
 Terminating at known equilibrium

Phase region boundary 27 at: 3.650E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated.. 14 equilibria  
 Terminating at known equilibrium

Phase region boundary 28 at: 7.919E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated 10 equilibria

Phase region boundary 29 at: 7.919E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated.. 3 equilibria  
 Terminating at known equilibrium

Phase region boundary 30 at: 7.919E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated.. 10 equilibria  
 Terminating at known equilibrium

Phase region boundary 31 at: 2.445E-01 1.230E+03  
 \*\* LIQUID  
 BCC  
 Calculated.. 4 equilibria  
 Terminating at known equilibrium

Phase region boundary 32 at: 2.445E-01 1.230E+03  
 \*\* LIQUID  
 BCC  
 Calculated 26 equilibria

Phase region boundary 33 at: 8.860E-01 1.230E+03  
 \*\* LIQUID  
 FCC  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium

Phase region boundary 34 at: 8.860E-01 1.230E+03  
 \*\* LIQUID  
 FCC  
 Calculated 29 equilibria

Phase region boundary 35 at: 6.399E-03 1.397E+03  
 LIQUID  
 \*\* BCC  
 Calculated 10 equilibria

Phase region boundary 36 at: 6.399E-03 1.397E+03  
 LIQUID  
 \*\* BCC  
 Calculated.. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 37 at: 2.293E-01 1.244E+03  
 LIQUID  
 \*\* BCC  
 Calculated 21 equilibria

Phase region boundary 38 at: 2.293E-01 1.244E+03  
 LIQUID  
 \*\* BCC  
 Calculated.. 4 equilibria  
 Terminating at known equilibrium

Phase region boundary 39 at: 6.122E-01 1.242E+03  
 LIQUID  
 \*\* A2B  
 Calculated.. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 40 at: 6.122E-01 1.242E+03  
 LIQUID  
 \*\* A2B  
 Calculated.. 8 equilibria  
 Terminating at known equilibrium

Phase region boundary 41 at: 9.927E-01 1.613E+03  
 LIQUID

```

** FCC
Calculated.                20 equilibria
Terminating at known equilibrium

Phase region boundary 42 at:  9.927E-01  1.613E+03
LIQUID
** FCC
Calculated                12 equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tce
x36.POLY3
CPU time for mapping          1 seconds
POLY_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

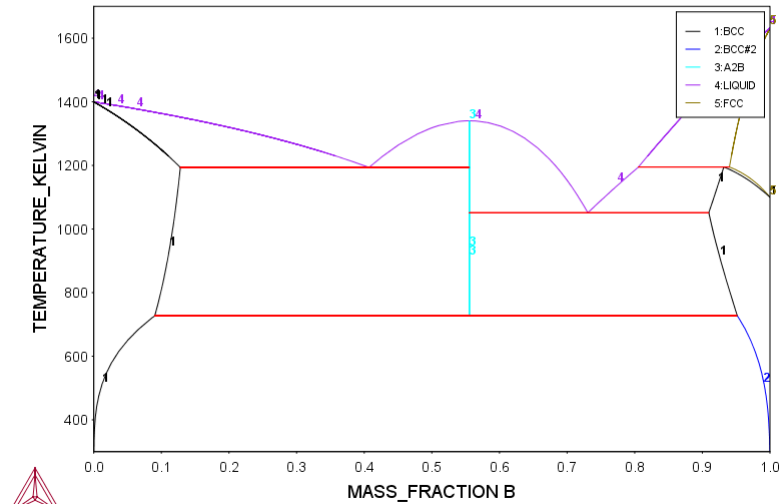
```

Setting automatic diagram axes

```

POST: s-l d
... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
... the command in full is PLOT DIAGRAM
2016.05.16.14.20.30
A,B
P=1E5,N=1

```



```

POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:Hit RETURN to continue
POST: ba
... the command in full is BACK
POLY_3: ba
... the command in full is BACK

```

PARROT VERSION 5.3

```

Global minimization used as test only
PARROT: @@ Now there is an equilibrium between fcc, bcc and liquid at high B
PARROT: @@ restore equilibrium 4 on the POP file
PARROT: ed
... the command in full is EDIT_EXPERIMENTS
ED_EXP: read 1
... the command in full is READ_WORKSPACES
ED_EXP: s-e 4
... the command in full is SELECT_EQUILIBRIUM
Equilibrium number      4 , label AINV
ED_EXP: s-we 1
... the command in full is SET_WEIGHT
Equilibria (range) or label(s) /PRESENT/: PRESENT
ED_EXP: s-a-s
... the command in full is SET_ALL_START_VALUES
T /1204.671469/: 1200
Automatic start values for phase constituents? /N/: N

```

```

Phase LIQUID
Major constituent(s) /b/: b

```

```

Phase BCC
Major constituent(s) /b/: b

```

```

Phase FCC
Major constituent(s) /b/: b

```

```

ED_EXP:
ED_EXP: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Testing result with global minimization
14 ITS, CPU TIME USED 0 SECONDS

```

```

ED_EXP: l-e
... the command in full is LIST_EQUILIBRIUM

```

OUTPUT TO SCREEN OR FILE /SCREEN/:

```

Options /VWCS/: VWCS
Output from POLY-3, equilibrium = 4, label AINV, database:

```

```

Conditions:
P=1.01325E5
FIXED PHASES
LIQUID=1 BCC=1 FCC=1
DEGREES OF FREEDOM 0

Temperature 1195.10 K ( 921.95 C), Pressure 1.013250E+05
Number of moles of components 3.00000E+00, Mass in grams 1.29944E+02
Total Gibbs energy -9.43346E+03, Enthalpy 1.97100E+04, Volume 0.00000E+00

```

```

Component      Moles      W-Fraction  Activity   Potential  Ref.stat
A               6.6854E-01  1.0290E-01  4.0783E-01 -8.9123E+03 SER
B               2.3315E+00  8.9710E-01  8.6070E-01 -1.4906E+03 SER

FCC              Status FIXED      Driving force  0.0000E+00
Moles 1.0000E+00, Mass 4.5876E+01, Volume fraction 0.0000E+00 Mass fractions:
B 9.40072E-01 A 5.99283E-02

BCC              Status FIXED      Driving force  0.0000E+00
Moles 1.0000E+00, Mass 4.5360E+01, Volume fraction 0.0000E+00 Mass fractions:
B 9.31812E-01 A 6.81875E-02

LIQUID           Status FIXED      Driving force  0.0000E+00
Moles 1.0000E+00, Mass 3.8707E+01, Volume fraction 0.0000E+00 Mass fractions:
B 8.05502E-01 A 1.94498E-01

EXPERIMENT T=1203:DT $1195.1:10 NO=1
EXPERIMENT W(LIQUID,A)=0.19:DX $0.194498:2E-2 NO=2
EXPERIMENT W(BCC,A)=6.9E-2:DX $6.81875E-2:2E-2 NO=3
EXPERIMENT W(FCC,A)=6E-2:DX $5.99283E-2:2E-2 NO=4
ED_EXP: @@ Now equilibrium 4 is on the high B side
ED_EXP: save
... the command in full is SAVE_WORKSPACES
ED_EXP: ba
... the command in full is BACK
PARROT: resc
... the command in full is RESCALE_VARIABLES
PARROT: opt 0
... the command in full is OPTIMIZE_VARIABLES
Use 29 experiments, maximum is 2000
Use 554 real workspace, maximum is 50000
PARROT: l-r C SCREEN
... the command in full is LIST_RESULT

=====
OUTPUT FROM P A R R O T. DATE 2016. 5.16 14:20:31

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 0

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 0 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.  VALUE      START VALUE      SCALING FACTOR      REL.STAND.DEV
V1    2.01820918E+04  2.01820918E+04  2.01820918E+04  0.00000000E+00
V2    -2.90936108E+01 -2.90936108E+01 -2.90936108E+01  0.00000000E+00
V11   -2.18127452E+04  1.55559572E+01
V12    1.55559572E+01  2.36701045E+04  2.36701045E+04  0.00000000E+00
V15    2.36701045E+04  -7.56540324E+00 -7.56540324E+00  0.00000000E+00
V16    -7.56540324E+00 -7.56540324E+00 -7.56540324E+00  0.00000000E+00
V17    3.00342248E+03  3.00342248E+03  3.00342248E+03  0.00000000E+00
V19    2.20133196E+04  2.20133196E+04  2.20133196E+04  0.00000000E+00
V20    -6.72497818E+00 -6.72497818E+00 -6.72497818E+00  0.00000000E+00

NUMBER OF OPTIMIZING VARIABLES : 7
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 0.00000000E+00 TO 8.21413189E-01
DEGREES OF FREEDOM 22. REDUCED SUM OF SQUARES 3.73369632E-02

$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS
DX=2E-2, P0=101325, DH=500, DT=10
DEFINED FUNCTIONS AND VARIABLES%
HTR=HM(LIQUID)-HM(A2B)
1 T=1193 1194. 10.0 0.6681 6.6807E-02
1 W(LIQUID,B)=0.408 0.4071 2.00E-02 -8.9916E-04 -4.4958E-02
1 W(BCC,B)=0.13 0.1280 2.00E-02 -1.9512E-03 -9.7560E-02
2 T=1341 1340. 10.0 -0.6301 -6.3010E-02
2 HTR=3727 3759. 5.00E+02 31.69 6.3385E-02
3 T=1049 1051. 10.0 2.137 0.2137
3 W(LIQUID,A)=0.27 0.2695 2.00E-02 -5.4230E-04 -2.7115E-02
3 W(BCC,A)=9.3E-2 9.0569E-02 2.00E-02 -2.4311E-03 -0.1216
4 T=1203 1195. 10.0 -7.904 -0.7904
4 W(LIQUID,A)=0.19 0.1945 2.00E-02 4.4979E-03 0.2249
4 W(BCC,A)=6.9E-2 6.8188E-02 2.00E-02 -8.1248E-04 -4.0624E-02
4 W(FCC,A)=6E-2 5.9928E-02 2.00E-02 -7.1681E-05 -3.5840E-03
5 T=726 727.5 10.0 1.501 0.1501
5 X(BCC,B)=3.7E-2 3.8199E-02 2.00E-02 1.1988E-03 5.9941E-02
5 X(BCC#2,A)=0.114 0.1128 2.00E-02 -1.1687E-03 -5.8436E-02
6 X(BCC,B)=3.7E-2 3.7779E-02 2.00E-02 7.7870E-04 3.8935E-02
6 X(BCC#2,A)=0.114 0.1118 2.00E-02 -2.1691E-03 -0.1085
10 W(LIQUID,A)=2E-2 1.9541E-02 2.00E-02 -4.5856E-04 -2.2928E-02
11 W(LIQUID,A)=4.2E-2 4.1844E-02 2.00E-02 -1.5590E-04 -7.7951E-03
12 W(LIQUID,A)=6.5E-2 6.4983E-02 2.00E-02 -1.6862E-05 -8.4310E-04
13 W(LIQUID,A)=9.3E-2 9.2906E-02 2.00E-02 -9.3697E-05 -4.6848E-03
20 W(LIQUID,A)=0.104 0.1041 2.00E-02 6.5965E-05 3.2982E-03
20 W(FCC,A)=3.8E-2 3.7928E-02 2.00E-02 -7.1810E-05 -3.5905E-03
21 W(LIQUID,A)=0.136 0.1370 2.00E-02 9.7746E-04 4.8873E-02
21 W(FCC,A)=4.7E-2 4.6724E-02 2.00E-02 -2.7609E-04 -1.3805E-02
22 W(LIQUID,A)=0.187 0.1875 2.00E-02 5.0747E-04 2.5374E-02
22 W(FCC,A)=5.9E-2 5.8445E-02 2.00E-02 -5.5491E-04 -2.7745E-02
23 W(LIQUID,A)=0.245 0.2448 2.00E-02 -1.5069E-04 -7.5343E-03
23 W(BCC,A)=8.5E-2 8.2833E-02 2.00E-02 -2.1672E-03 -0.1084

```

```
PARROT:
PARROT:Hit RETURN to continue
PARROT: opt 30
... the command in full is OPTIMIZE_VARIABLES
Use      29 experiments, maximum is      2000
Use     554 real workspace, maximum is    50000
The following output is provided by subroutine VA05A

      AT THE      0 TH ITERATION WE HAVE THE SUM OF SQUARES      8.21413189E-01
1 1.0000E+00      2 1.0000E+00      3 1.0000E+00      4 1.0000E+00      5 1.0000E+00
6 1.0000E+00      7 1.0000E+00

      AT THE      1 ST ITERATION WE HAVE THE SUM OF SQUARES      8.22231515E-01
1 1.0001E+00      2 1.0000E+00      3 1.0000E+00      4 1.0000E+00      5 1.0000E+00
6 1.0000E+00      7 1.0000E+00

      AT THE      2 ND ITERATION WE HAVE THE SUM OF SQUARES      8.24025606E-01
1 1.0000E+00      2 1.0001E+00      3 1.0000E+00      4 1.0000E+00      5 1.0000E+00
6 1.0000E+00      7 1.0000E+00

      AT THE      3 RD ITERATION WE HAVE THE SUM OF SQUARES      8.41459883E-01
1 1.0000E+00      2 1.0000E+00      3 1.0001E+00      4 1.0000E+00      5 1.0000E+00
6 1.0000E+00      7 1.0000E+00

      AT THE      4 TH ITERATION WE HAVE THE SUM OF SQUARES      8.13854563E-01
1 1.0000E+00      2 1.0000E+00      3 1.0000E+00      4 1.0001E+00      5 1.0000E+00
6 1.0000E+00      7 1.0000E+00

      AT THE      5 TH ITERATION WE HAVE THE SUM OF SQUARES      8.12128638E-01
1 1.0000E+00      2 1.0000E+00      3 1.0000E+00      4 1.0001E+00      5 1.0001E+00
6 1.0000E+00      7 1.0000E+00

      AT THE      6 TH ITERATION WE HAVE THE SUM OF SQUARES      7.96555860E-01
1 1.0000E+00      2 1.0000E+00      3 1.0000E+00      4 1.0001E+00      5 1.0001E+00
6 1.0001E+00      7 1.0000E+00

      AT THE      7 TH ITERATION WE HAVE THE SUM OF SQUARES      8.02217370E-01
1 1.0000E+00      2 1.0000E+00      3 1.0000E+00      4 1.0001E+00      5 1.0001E+00
6 1.0001E+00      7 1.0001E+00

      AT THE      8 TH ITERATION WE HAVE THE SUM OF SQUARES      2.23904464E-01
1 1.0000E+00      2 1.0000E+00      3 9.9684E-01      4 1.0013E+00      5 1.0004E+00
6 1.0026E+00      7 9.9908E-01

      AT THE      9 TH ITERATION WE HAVE THE SUM OF SQUARES      2.14217788E-01
1 1.0000E+00      2 9.9989E-01      3 9.9763E-01      4 1.0026E+00      5 1.0012E+00
6 1.0043E+00      7 1.0027E+00

      AT THE     10 TH ITERATION WE HAVE THE SUM OF SQUARES      2.02688406E-01
1 1.0001E+00      2 1.0000E+00      3 9.9857E-01      4 1.0047E+00      5 1.0024E+00
6 1.0073E+00      7 1.0104E+00

      AT THE     11 TH ITERATION WE HAVE THE SUM OF SQUARES      1.86054744E-01
1 1.0003E+00      2 1.0001E+00      3 1.0009E+00      4 1.0098E+00      5 1.0054E+00
6 1.0128E+00      7 1.0246E+00

      AT THE     12 TH ITERATION WE HAVE THE SUM OF SQUARES      1.70130539E-01
1 1.0007E+00      2 1.0004E+00      3 1.0050E+00      4 1.0192E+00      5 1.0109E+00
6 1.0237E+00      7 1.0537E+00

      AT THE     13 TH ITERATION WE HAVE THE SUM OF SQUARES      1.67854613E-01
1 1.0010E+00      2 1.0005E+00      3 1.0074E+00      4 1.0249E+00      5 1.0142E+00
6 1.0289E+00      7 1.0677E+00

      THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED      13 iterations
1 1.0010E+00      2 1.0005E+00      3 1.0074E+00      4 1.0249E+00      5 1.0142E+00
6 1.0289E+00      7 1.0677E+00

1 6.3161E-02      2 -3.7856E-02      3 -8.1409E-02      4 -6.8335E-02      5 4.9923E-02
6 2.5923E-01      7 -1.3946E-02      8 -9.1405E-02      9 -1.3190E-02     10 4.3922E-02
11 -6.3822E-02     12 -8.0234E-02     13 1.6660E-01     14 3.1149E-02     15 -6.4319E-02
16 8.0802E-03     17 -1.1993E-01     18 -1.7511E-02     19 4.0026E-04     20 7.0615E-03
21 -6.1522E-04     22 4.9462E-03     23 -1.7573E-03     24 4.0977E-02     25 -2.3417E-02
26 -2.5370E-03     27 -6.9024E-02     28 2.0311E-02     29 -7.1934E-02

      THE SUM OF SQUARES IS      1.67854613E-01
PARROT: l-r C SCREEN
... the command in full is LIST_RESULT

=====
OUTPUT FROM P A R R O T. DATE 2016. 5.16 14:20:31

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 14

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.  VALUE          START VALUE      SCALING FACTOR    REL.STAND.DEV
V1    2.02022854E+04   2.01820918E+04   2.01820918E+04   2.48851232E-02
V2    -2.91083428E+01  -2.90936108E+01  -2.90936108E+01  1.36093012E-02
V11   -2.18127452E+04
V12   1.55559572E+01
V15   2.38442417E+04   2.36701045E+04   2.36701045E+04   8.28181589E-02
V16   -7.75412305E+00  -7.56540324E+00  -7.56540324E+00  2.55327975E-01
```

```
V17      3.04598820E+03      3.00342248E+03      3.00342248E+03      2.36433798E-01
V19      2.26500827E+04      2.20133196E+04      2.20133196E+04      4.73555705E-01
V20     -7.18046737E+00     -6.72497818E+00     -6.72497818E+00      1.24878491E+00
```

```
NUMBER OF OPTIMIZING VARIABLES :    7
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM    8.21413188E-01 TO    1.67854613E-01
DEGREES OF FREEDOM    22. REDUCED SUM OF SQUARES    7.62975513E-03
```

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS

DX=2E-2, P0=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%

HTR=HM(LIQUID)-HM(A2B)

```
1 T=1193      1194.      10.0      0.6316      6.3161E-02
1 W(LIQUID,B)=0.408      0.4072      2.00E-02      -7.5711E-04      -3.7856E-02
1 W(BCC,B)=0.13      0.1284      2.00E-02      -1.6282E-03      -8.1409E-02
2 T=1341      1340.      10.0      -0.6833      -6.8335E-02
2 HTR=3727      3752.      5.00E+02      24.96      4.9923E-02
3 T=1049      1052.      10.0      2.592      0.2592
3 W(LIQUID,A)=0.27      0.2697      2.00E-02      -2.7892E-04      -1.3946E-02
3 W(BCC,A)=9.3E-2      9.1172E-02      2.00E-02      -1.8281E-03      -9.1405E-02
4 T=1203      1203.      10.0      -0.1319      -1.3190E-02
4 W(LIQUID,A)=0.19      0.1909      2.00E-02      8.7843E-04      4.3922E-02
4 W(BCC,A)=6.9E-2      6.7724E-02      2.00E-02      -1.2764E-03      -6.3822E-02
4 W(FCC,A)=6E-2      5.8395E-02      2.00E-02      -1.6047E-03      -8.0234E-02
5 T=726      727.7      10.0      1.666      0.1666
5 X(BCC,B)=3.7E-2      3.7623E-02      2.00E-02      6.2299E-04      3.1149E-02
5 X(BCC#2,A)=0.114      0.1127      2.00E-02      -1.2864E-03      -6.4319E-02
6 X(BCC,B)=3.7E-2      3.7162E-02      2.00E-02      1.6160E-04      8.0802E-03
6 X(BCC#2,A)=0.114      0.1116      2.00E-02      -2.3986E-03      -0.1199
10 W(LIQUID,A)=2E-2      1.9650E-02      2.00E-02      -3.5022E-04      -1.7511E-02
11 W(LIQUID,A)=4.2E-2      4.2008E-02      2.00E-02      8.0052E-06      4.0026E-04
12 W(LIQUID,A)=6.5E-2      6.5141E-02      2.00E-02      1.4123E-04      7.0615E-03
13 W(LIQUID,A)=9.3E-2      9.2988E-02      2.00E-02      -1.2304E-05      -6.1522E-04
20 W(LIQUID,A)=0.104      0.1041      2.00E-02      9.8925E-05      4.9462E-03
20 W(FCC,A)=3.8E-2      3.7965E-02      2.00E-02      -3.5145E-05      -1.7573E-03
21 W(LIQUID,A)=0.136      0.1368      2.00E-02      8.1954E-04      4.0977E-02
21 W(FCC,A)=4.7E-2      4.6532E-02      2.00E-02      -4.6834E-04      -2.3417E-02
22 W(LIQUID,A)=0.187      0.1869      2.00E-02      -5.0739E-05      -2.5370E-03
22 W(FCC,A)=5.9E-2      5.7620E-02      2.00E-02      -1.3805E-03      -6.9024E-02
23 W(LIQUID,A)=0.245      0.2454      2.00E-02      4.0622E-04      2.0311E-02
23 W(BCC,A)=8.5E-2      8.3561E-02      2.00E-02      -1.4387E-03      -7.1934E-02
```

PARROT:

PARROT:

PARROT:Hit RETURN to continue

PARROT: @@ Now optimize all parameters and all experiments

PARROT: l-a-v

... the command in full is LIST\_ALL\_VARIABLES

OUTPUT TO SCREEN OR FILE /SCREEN/:

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.02022854E+04	2.01820918E+04	2.01820918E+04	2.48851232E-02
V2	-2.91083428E+01	-2.90936108E+01	-2.90936108E+01	1.36093012E-02
V11	-2.18127452E+04			
V12	1.55559572E+01			
V15	2.38442417E+04	2.36701045E+04	2.36701045E+04	8.28181589E-02
V16	-7.75412305E+00	-7.56540324E+00	-7.56540324E+00	2.55327975E-01
V17	3.04598820E+03	3.00342248E+03	3.00342248E+03	2.36433798E-01
V19	2.26500827E+04	2.20133196E+04	2.20133196E+04	4.73555705E-01
V20	-7.18046737E+00	-6.72497818E+00	-6.72497818E+00	1.24878491E+00

```
NUMBER OF OPTIMIZING VARIABLES :    7
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM    8.21413188E-01 TO    1.67854613E-01
DEGREES OF FREEDOM    22. REDUCED SUM OF SQUARES    7.62975513E-03
```

PARROT: s-o-v 11-12

... the command in full is SET\_OPTIMIZING\_VARIABLE

PARROT: ed

... the command in full is EDIT\_EXPERIMENTS

ED\_EXP: read 1

... the command in full is READ\_WORKSPACES

ED\_EXP: c-a

... the command in full is COMPUTE\_ALL\_EQUILIBRIA

Eq	Lab	Iter	Weight	Temp	Exp	Fix	phases	or comments
1	AINV	2	1.	1193.6			LIQUID A2B BCC	
2	AINV	2	1.	1340.3			LIQUID A2B	
3	AINV	2	1.	1051.6			LIQUID A2B BCC	
4	AINV	2	1.	1202.9			LIQUID BCC FCC	
5	AINV	2	1.	727.7			A2B BCC BCC#2	
6	AINV	2	1.	726.0			BCC BCC#2	
10	ALF	2	1.	1594.0			LIQUID FCC	
11	ALF	2	1.	1548.0			LIQUID FCC	
12	ALF	2	1.	1499.0			LIQUID FCC	
13	ALF	2	1.	1438.0			LIQUID FCC	
20	ATIE	2	1.	1413.0			LIQUID FCC	
21	ATIE	2	1.	1337.0			LIQUID FCC	
22	ATIE	2	1.	1213.0			LIQUID FCC	
23	ATIE	2	1.	1100.0			LIQUID BCC	
100	AA	< unused >		1573.0			LIQUID	
101	AA	< unused >		1573.0			LIQUID	
102	AA	< unused >		1573.0			LIQUID	
103	AA	< unused >		1573.0			LIQUID	
104	AA	< unused >		1573.0			LIQUID	
105	AA	< unused >		1573.0			LIQUID	
106	AA	< unused >		1573.0			LIQUID	
107	AA	< unused >		1573.0			LIQUID	
108	AA	< unused >		1573.0			LIQUID	
110	AH	< unused >		1773.0			LIQUID	
111	AH	< unused >		1773.0			LIQUID	
112	AH	< unused >		1773.0			LIQUID	
113	AH	< unused >		1773.0			LIQUID	
114	AH	< unused >		1773.0			LIQUID	
115	AH	< unused >		1773.0			LIQUID	
116	AH	< unused >		1773.0			LIQUID	
117	AH	< unused >		1773.0			LIQUID	

```

118 AH < unused > 1773.0 LIQUID
ED_EXP: s-we 1 100-118
... the command in full is SET_WEIGHT
ED_EXP: s-e 1
... the command in full is SELECT_EQUILIBRIUM
Equilibrium number 1 , label AINV
ED_EXP: c-a
... the command in full is COMPUTE_ALL_EQUILIBRIA
Eq Lab Iter Weight Temp Exp Fix phases or comments
1 AINV 2 1. 1193.6 LIQUID A2B BCC
2 AINV 2 1. 1340.3 LIQUID A2B
3 AINV 2 1. 1051.6 LIQUID A2B BCC
4 AINV 2 1. 1202.9 LIQUID BCC FCC
5 AINV 2 1. 727.7 A2B BCC BCC#2
6 AINV 2 1. 726.0 BCC BCC#2
10 ALF 2 1. 1594.0 LIQUID FCC
11 ALF 2 1. 1548.0 LIQUID FCC
12 ALF 2 1. 1499.0 LIQUID FCC
13 ALF 2 1. 1438.0 LIQUID FCC
20 ATIE 2 1. 1413.0 LIQUID FCC
21 ATIE 2 1. 1337.0 LIQUID FCC
22 ATIE 2 1. 1213.0 LIQUID FCC
23 ATIE 2 1. 1100.0 LIQUID BCC
100 AA 2 1. 1573.0 LIQUID
101 AA 2 1. 1573.0 LIQUID
102 AA 2 1. 1573.0 LIQUID
103 AA 2 1. 1573.0 LIQUID
104 AA 2 1. 1573.0 LIQUID
105 AA 2 1. 1573.0 LIQUID
106 AA 2 1. 1573.0 LIQUID
107 AA 2 1. 1573.0 LIQUID
108 AA 2 1. 1573.0 LIQUID
110 AH 2 1. 1773.0 LIQUID
111 AH 2 1. 1773.0 LIQUID
112 AH 2 1. 1773.0 LIQUID
113 AH 2 1. 1773.0 LIQUID
114 AH 2 1. 1773.0 LIQUID
115 AH 2 1. 1773.0 LIQUID
116 AH 2 1. 1773.0 LIQUID
117 AH 2 1. 1773.0 LIQUID
118 AH 2 1. 1773.0 LIQUID
ED_EXP: save
... the command in full is SAVE_WORKSPACES
ED_EXP: ba
... the command in full is BACK
PARROT: opt 30
... the command in full is OPTIMIZE_VARIABLES
Use 47 experiments, maximum is 2000
Use 1082 real workspace, maximum is 50000
The following output is provided by subroutine VA05A

```

```

      AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 5.15879918E-01
1 1.0010E+00 2 1.0005E+00 3 1.0000E+00 4 1.0000E+00 5 1.0074E+00
6 1.0249E+00 7 1.0142E+00 8 1.0289E+00 9 1.0677E+00

      AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 5.16684214E-01
1 1.0011E+00 2 1.0005E+00 3 1.0000E+00 4 1.0000E+00 5 1.0074E+00
6 1.0249E+00 7 1.0142E+00 8 1.0289E+00 9 1.0677E+00

      AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 5.18528647E-01
1 1.0010E+00 2 1.0006E+00 3 1.0000E+00 4 1.0000E+00 5 1.0074E+00
6 1.0249E+00 7 1.0142E+00 8 1.0289E+00 9 1.0677E+00

      AT THE 3 RD ITERATION WE HAVE THE SUM OF SQUARES 5.10059302E-01
1 1.0010E+00 2 1.0005E+00 3 1.0001E+00 4 1.0000E+00 5 1.0074E+00
6 1.0249E+00 7 1.0142E+00 8 1.0289E+00 9 1.0677E+00

      AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 5.14690131E-01
1 1.0010E+00 2 1.0005E+00 3 1.0001E+00 4 1.0001E+00 5 1.0074E+00
6 1.0249E+00 7 1.0142E+00 8 1.0289E+00 9 1.0677E+00

      AT THE 5 TH ITERATION WE HAVE THE SUM OF SQUARES 5.10340685E-01
1 1.0010E+00 2 1.0005E+00 3 1.0001E+00 4 1.0000E+00 5 1.0075E+00
6 1.0249E+00 7 1.0142E+00 8 1.0289E+00 9 1.0677E+00

      AT THE 6 TH ITERATION WE HAVE THE SUM OF SQUARES 5.10048087E-01
1 1.0010E+00 2 1.0005E+00 3 1.0001E+00 4 1.0000E+00 5 1.0074E+00
6 1.0250E+00 7 1.0142E+00 8 1.0289E+00 9 1.0677E+00

      AT THE 7 TH ITERATION WE HAVE THE SUM OF SQUARES 5.10055130E-01
1 1.0010E+00 2 1.0005E+00 3 1.0001E+00 4 1.0000E+00 5 1.0074E+00
6 1.0250E+00 7 1.0143E+00 8 1.0289E+00 9 1.0677E+00

      AT THE 8 TH ITERATION WE HAVE THE SUM OF SQUARES 5.10212338E-01
1 1.0010E+00 2 1.0005E+00 3 1.0001E+00 4 1.0000E+00 5 1.0074E+00
6 1.0250E+00 7 1.0142E+00 8 1.0290E+00 9 1.0677E+00

      AT THE 9 TH ITERATION WE HAVE THE SUM OF SQUARES 5.10033022E-01
1 1.0010E+00 2 1.0005E+00 3 1.0001E+00 4 1.0000E+00 5 1.0074E+00
6 1.0250E+00 7 1.0142E+00 8 1.0289E+00 9 1.0678E+00

      AT THE 10 TH ITERATION WE HAVE THE SUM OF SQUARES 4.31534544E-01
1 1.0007E+00 2 1.0011E+00 3 1.0017E+00 4 9.9872E-01 5 1.0073E+00
6 1.0251E+00 7 1.0142E+00 8 1.0289E+00 9 1.0678E+00

      AT THE 11 TH ITERATION WE HAVE THE SUM OF SQUARES 3.88006645E-01
1 1.0007E+00 2 1.0016E+00 3 1.0015E+00 4 9.9831E-01 5 1.0076E+00
6 1.0269E+00 7 1.0145E+00 8 1.0283E+00 9 1.0674E+00

      AT THE 12 TH ITERATION WE HAVE THE SUM OF SQUARES 3.46571329E-01
1 1.0012E+00 2 1.0021E+00 3 1.0017E+00 4 9.9707E-01 5 1.0078E+00
6 1.0307E+00 7 1.0152E+00 8 1.0271E+00 9 1.0665E+00

      AT THE 13 TH ITERATION WE HAVE THE SUM OF SQUARES 2.88315117E-01
1 1.0019E+00 2 1.0031E+00 3 1.0011E+00 4 9.9524E-01 5 1.0092E+00
6 1.0382E+00 7 1.0164E+00 8 1.0246E+00 9 1.0647E+00

      AT THE 14 TH ITERATION WE HAVE THE SUM OF SQUARES 2.01092406E-01
1 1.0035E+00 2 1.0050E+00 3 1.0003E+00 4 9.9135E-01 5 1.0119E+00
6 1.0533E+00 7 1.0190E+00 8 1.0194E+00 9 1.0612E+00

      AT THE 15 TH ITERATION WE HAVE THE SUM OF SQUARES 9.39326709E-02
1 1.0066E+00 2 1.0086E+00 3 9.9812E-01 4 9.8393E-01 5 1.0177E+00
6 1.0836E+00 7 1.0240E+00 8 1.0095E+00 9 1.0548E+00

```

```

      AT THE 16 TH ITERATION WE HAVE THE SUM OF SQUARES 6.73924422E-02
1 1.0093E+00 2 1.0115E+00 3 9.9634E-01 4 9.7778E-01 5 1.0224E+00
6 1.1084E+00 7 1.0281E+00 8 1.0021E+00 9 1.0514E+00

      THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 16 iterations
1 1.0093E+00 2 1.0115E+00 3 9.9634E-01 4 9.7778E-01 5 1.0224E+00
6 1.1084E+00 7 1.0281E+00 8 1.0021E+00 9 1.0514E+00

1 -5.7709E-02 2 -9.3404E-03 3 1.4435E-02 4 2.0965E-02 5 -2.5772E-02
6 -5.2196E-02 7 1.9264E-02 8 2.6907E-02 9 1.1430E-02 10 2.7509E-02
11 8.8336E-03 12 1.3392E-02 13 -4.8280E-02 14 2.2178E-02 15 5.2234E-03
16 2.9005E-02 17 2.1915E-02 18 -2.1795E-02 19 -7.8107E-03 20 -4.4451E-03
21 -1.5094E-02 22 -1.0366E-02 23 1.5822E-02 24 2.4683E-02 25 1.5219E-02
26 -1.4822E-02 27 2.0407E-02 28 -1.2809E-02 29 1.5407E-02 30 -9.5946E-03
31 -1.6846E-02 32 2.7408E-02 33 8.6976E-02 34 1.2428E-01 35 1.0162E-01
36 -1.7386E-02 37 7.0520E-02 38 -1.9513E-02 39 1.6094E-02 40 4.5500E-02
41 4.8219E-02 42 4.6251E-02 43 4.1594E-02 44 3.4251E-02 45 2.2219E-02
46 7.5004E-03 47 -1.1906E-02
```

THE SUM OF SQUARES IS 6.73924422E-02

PARROT: l-r C SCREEN  
... the command in full is LIST\_RESULT

=====

OUTPUT FROM P A R R O T. DATE 2016. 5.16 14:20:31

\*\*\* SUCCESSFUL OPTIMIZATION. \*\*\*  
NUMBER OF ITERATIONS: 17

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N  
MINIMUM SAVE ON FILE: Y  
ERROR FOR INEQUALITIES = 1.00000000E+00  
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04  
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)  
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04  
ACC = (INITIAL SUM OF SQUARES) \* 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.03691169E+04	2.01820918E+04	2.01820918E+04	3.02498426E-02
V2	-2.94290453E+01	-2.90936108E+01	-2.90936108E+01	2.30117855E-02
V11	-2.17328114E+04	-2.18127452E+04	-2.18127452E+04	3.47139484E-02
V12	1.52102756E+01	1.55559572E+01	1.55559572E+01	5.38555420E-02
V15	2.42012673E+04	2.36701045E+04	2.36701045E+04	8.60926362E-02
V16	-8.38545778E+00	-7.56540324E+00	-7.56540324E+00	2.83695736E-01
V17	3.08774252E+03	3.00342248E+03	3.00342248E+03	2.37803227E-01
V19	2.20600539E+04	2.20133196E+04	2.20133196E+04	4.87694893E-01
V20	-7.07096129E+00	-6.72497818E+00	-6.72497818E+00	1.27666199E+00

NUMBER OF OPTIMIZING VARIABLES : 9  
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO  
THE SUM OF SQUARES HAS CHANGED FROM 5.15879918E-01 TO 6.73924422E-02  
DEGREES OF FREEDOM 38. REDUCED SUM OF SQUARES 1.77348532E-03

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS

DX=2E-2, P0=101325, DH=500, DT=10  
DEFINED FUNCTIONS AND VARIABLES%

HTR=HM(LIQUID)-HM(A2B)

1 T=1193	1192.	10.0	-0.5771	-5.7709E-02
1 W(LIQUID,B)=0.408	0.4078	2.00E-02	-1.8681E-04	-9.3404E-03
1 W(BCC,B)=0.13	0.1303	2.00E-02	2.8870E-04	1.4435E-02
2 T=1341	1341.	10.0	0.2096	2.0965E-02
2 HTR=3727	3714.	5.00E+02	-12.89	-2.5772E-02
3 T=1049	1048.	10.0	-0.5220	-5.2196E-02
3 W(LIQUID,A)=0.27	0.2704	2.00E-02	3.8528E-04	1.9264E-02
3 W(BCC,A)=9.3E-2	9.3538E-02	2.00E-02	5.3815E-04	2.6907E-02
4 T=1203	1203.	10.0	0.1143	1.1430E-02
4 W(LIQUID,A)=0.19	0.1906	2.00E-02	5.5018E-04	2.7509E-02
4 W(BCC,A)=6.9E-2	6.9177E-02	2.00E-02	1.7667E-04	8.8336E-03
4 W(FCC,A)=6E-2	6.0268E-02	2.00E-02	2.6783E-04	1.3392E-02
5 T=726	725.5	10.0	-0.4828	-4.8280E-02
5 X(BCC,B)=3.7E-2	3.7444E-02	2.00E-02	4.4356E-04	2.2178E-02
5 X(BCC#2,A)=0.114	0.1141	2.00E-02	1.0447E-04	5.2234E-03
6 X(BCC,B)=3.7E-2	3.7580E-02	2.00E-02	5.8011E-04	2.9005E-02
6 X(BCC#2,A)=0.114	0.1144	2.00E-02	4.3830E-04	2.1915E-02
10 W(LIQUID,A)=2E-2	1.9564E-02	2.00E-02	-4.3589E-04	-2.1795E-02
11 W(LIQUID,A)=4.2E-2	4.1844E-02	2.00E-02	-1.5621E-04	-7.8107E-03
12 W(LIQUID,A)=6.5E-2	6.4911E-02	2.00E-02	-8.8902E-05	-4.4451E-03
13 W(LIQUID,A)=9.3E-2	9.2698E-02	2.00E-02	-3.0187E-04	-1.5094E-02
20 W(LIQUID,A)=0.104	0.1038	2.00E-02	-2.0731E-04	-1.0366E-02
20 W(FCC,A)=3.8E-2	3.8316E-02	2.00E-02	3.1645E-04	1.5822E-02
21 W(LIQUID,A)=0.136	0.1365	2.00E-02	4.9366E-04	2.4683E-02
21 W(FCC,A)=4.7E-2	4.7304E-02	2.00E-02	3.0438E-04	1.5219E-02
22 W(LIQUID,A)=0.187	0.1867	2.00E-02	-2.9644E-04	-1.4822E-02
22 W(FCC,A)=5.9E-2	5.9408E-02	2.00E-02	4.0813E-04	2.0407E-02
23 W(LIQUID,A)=0.245	0.2447	2.00E-02	-2.5617E-04	-1.2809E-02
23 W(BCC,A)=8.5E-2	8.5308E-02	2.00E-02	3.0814E-04	1.5407E-02
100 ACR(B)=0.94	0.9397	2.85E-02	-2.7309E-04	-9.5946E-03
101 ACR(B)=0.84	0.8395	2.82E-02	-4.7482E-04	-1.6846E-02
102 ACR(B)=0.74	0.7408	2.81E-02	7.6893E-04	2.7408E-02
103 ACR(B)=0.64	0.6424	2.81E-02	2.4411E-03	8.6976E-02
104 ACR(B)=0.54	0.5435	2.82E-02	3.5079E-03	0.1243
105 ACR(B)=0.44	0.4429	2.85E-02	2.9003E-03	0.1016
106 ACR(B)=0.34	0.3395	2.90E-02	-5.0467E-04	-1.7386E-02
107 ACR(B)=0.23	0.2321	2.97E-02	2.0948E-03	7.0520E-02
108 ACR(B)=0.12	0.1194	3.06E-02	-5.9712E-04	-1.9513E-02
110 HMR(LIQUID)=-1964	-1956.	5.00E+02	8.047	1.6094E-02
111 HMR(LIQUID)=-3500	-3477.	5.00E+02	22.75	4.5500E-02
112 HMR(LIQUID)=-4588	-4564.	5.00E+02	24.11	4.8219E-02



113	HMR(LIQUID)=-5239	-5216.	5.00E+02	23.13	4.6251E-02
114	HMR(LIQUID)=-5454	-5433.	5.00E+02	20.80	4.1594E-02
115	HMR(LIQUID)=-5233	-5216.	5.00E+02	17.13	3.4251E-02
116	HMR(LIQUID)=-4575	-4564.	5.00E+02	11.11	2.2219E-02
117	HMR(LIQUID)=-3481	-3477.	5.00E+02	3.750	7.5004E-03
118	HMR(LIQUID)=-1950	-1956.	5.00E+02	-5.953	-1.1906E-02

```

PARROT:
PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ Calculate the phase diagram a final time.
PARROT: mac tcex36cpd
... the command in full is MACRO_FILE_OPEN
PARROT: set-echo
NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
... the command in full is GOTO_MODULE
POLY_3:
POLY_3: @@ In PARROT, the global minimization is turned off automatically.
POLY_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY_3: @@ message will be given.
POLY_3:
POLY_3: advanced-option global yes,,
... the command in full is ADVANCED_OPTIONS
Settings for global minimization:
*** WARNING *** Global equilibrium calculation may create new composition sets
and this may corrupt your PARROT work file (.PAR file).
Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY_3:
POLY_3: def-com,,,,
... the command in full is DEFINE_COMPONENTS
POLY_3: s-a-v 1 w(b) 0 1,,,,
... the command in full is SET_AXIS_VARIABLE
The condition W(B)=.1234 created
POLY_3: s-a-v 2 t 300 1700,,,,
... the command in full is SET_AXIS_VARIABLE
The condition T=942.2 created
POLY_3: s-c t=500
... the command in full is SET_CONDITION
POLY_3: l-c
... the command in full is LIST_CONDITIONS
W(B)=0.1234, P=1E5, N=1, T=500
DEGREES OF FREEDOM 0
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 412 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY_3: save tcex36 y
... the command in full is SAVE_WORKSPACES

```

This file contains results from a previous STEP or MAP command.  
The SAVE command will save the current status of the program but destroy  
the results from the previous STEP or MAP commands.

```

POLY_3: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

```

Organizing start points

Using ADDED start equilibria

```

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

```

```

Phase region boundary 1 at: 7.140E-01 3.100E+02
BCC
** BCC#2
Calculated.. 2 equilibria
Terminating at axis limit.

```

Phase region boundary 2 at: 7.141E-01 3.000E+02  
 BCC  
 \*\* BCC#2  
 Calculated. 14 equilibria

Phase region boundary 3 at: 6.819E-01 7.255E+02  
 \*\* A2B  
 BCC  
 \*\* BCC#2

Phase region boundary 4 at: 3.626E-01 7.255E+02  
 \*\* A2B  
 BCC  
 Calculated. 15 equilibria

Phase region boundary 5 at: 3.771E-01 1.192E+03  
 \*\* LIQUID  
 \*\* A2B  
 BCC

Phase region boundary 6 at: 2.828E-01 1.192E+03  
 \*\* LIQUID  
 BCC  
 Calculated 28 equilibria

Phase region boundary 7 at: 4.863E-01 1.192E+03  
 \*\* LIQUID  
 A2B  
 Calculated. 28 equilibria

Phase region boundary 8 at: 6.500E-01 1.048E+03  
 \*\* LIQUID  
 A2B  
 \*\* BCC

Phase region boundary 9 at: 7.639E-01 1.048E+03  
 A2B  
 \*\* BCC  
 Calculated. 11 equilibria  
 Terminating at known equilibrium

Phase region boundary 10 at: 8.273E-01 1.048E+03  
 LIQUID  
 \*\* BCC  
 Calculated. 8 equilibria

Phase region boundary 11 at: 8.748E-01 1.203E+03  
 LIQUID  
 \*\* BCC  
 \*\* FCC

Phase region boundary 12 at: 8.799E-01 1.203E+03  
 LIQUID  
 \*\* FCC  
 Calculated 35 equilibria

Phase region boundary 13 at: 9.353E-01 1.203E+03  
 BCC  
 \*\* FCC  
 Calculated 24 equilibria

Phase region boundary 14 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 15 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 16 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 17 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 18 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 19 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 20 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 21 at: 7.140E-01 3.100E+02  
 \*\* BCC  
 BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 22 at: 7.140E-01 3.100E+02  
 \*\* BCC  
 BCC#2

Calculated. 13 equilibria  
 Terminating at known equilibrium  
  
 Phase region boundary 23 at: 7.140E-01 3.100E+02  
 \*\* BCC  
 BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.  
  
 Phase region boundary 24 at: 7.140E-01 3.100E+02  
 \*\* BCC  
 BCC#2  
 Calculated. 13 equilibria  
 Terminating at known equilibrium  
  
 Phase region boundary 25 at: 3.647E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated 10 equilibria  
  
 Phase region boundary 26 at: 3.647E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated. 3 equilibria  
 Terminating at known equilibrium  
  
 Phase region boundary 27 at: 3.647E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated. 14 equilibria  
 Terminating at known equilibrium  
  
 Phase region boundary 28 at: 7.910E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated 10 equilibria  
  
 Phase region boundary 29 at: 7.910E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated. 3 equilibria  
 Terminating at known equilibrium  
  
 Phase region boundary 30 at: 7.910E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated. 9 equilibria  
 Terminating at known equilibrium  
  
 Phase region boundary 31 at: 2.448E-01 1.230E+03  
 \*\* LIQUID  
 BCC  
 Calculated. 4 equilibria  
 Terminating at known equilibrium  
  
 Phase region boundary 32 at: 2.448E-01 1.230E+03  
 \*\* LIQUID  
 BCC  
 Calculated 26 equilibria  
  
 Phase region boundary 33 at: 8.858E-01 1.230E+03  
 \*\* LIQUID  
 FCC  
 Calculated. 2 equilibria  
 Terminating at known equilibrium  
  
 Phase region boundary 34 at: 8.858E-01 1.230E+03  
 \*\* LIQUID  
 FCC  
 Calculated 29 equilibria  
  
 Phase region boundary 35 at: 6.415E-03 1.397E+03  
 LIQUID  
 \*\* BCC  
 Calculated 13 equilibria  
  
 Phase region boundary 36 at: 6.415E-03 1.397E+03  
 LIQUID  
 \*\* BCC  
 Calculated. 13 equilibria  
 Terminating at known equilibrium  
  
 Phase region boundary 37 at: 2.299E-01 1.244E+03  
 LIQUID  
 \*\* BCC  
 Calculated 23 equilibria  
  
 Phase region boundary 38 at: 2.299E-01 1.244E+03  
 LIQUID  
 \*\* BCC  
 Calculated. 4 equilibria  
 Terminating at known equilibrium  
  
 Phase region boundary 39 at: 6.122E-01 1.240E+03  
 LIQUID  
 \*\* A2B  
 Calculated. 14 equilibria  
 Terminating at known equilibrium  
  
 Phase region boundary 40 at: 6.122E-01 1.240E+03  
 LIQUID  
 \*\* A2B  
 Calculated. 8 equilibria  
 Terminating at known equilibrium  
  
 Phase region boundary 41 at: 9.927E-01 1.613E+03  
 LIQUID  
 \*\* FCC  
 Calculated. 20 equilibria  
 Terminating at known equilibrium  
  
 Phase region boundary 42 at: 9.927E-01 1.613E+03  
 LIQUID  
 \*\* FCC  
 Calculated 9 equilibria

```

*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tce
x36.POLY3
CPU time for mapping                      1 seconds
POLY_3: post

```

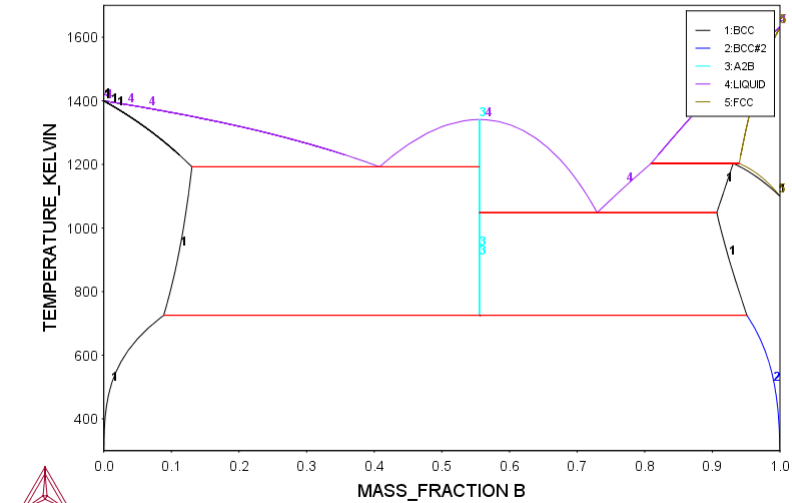
POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

```

POST: s-l d
... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
... the command in full is PLOT DIAGRAM
2016.05.16.14.20.34
A,B
P=1E5,N=1

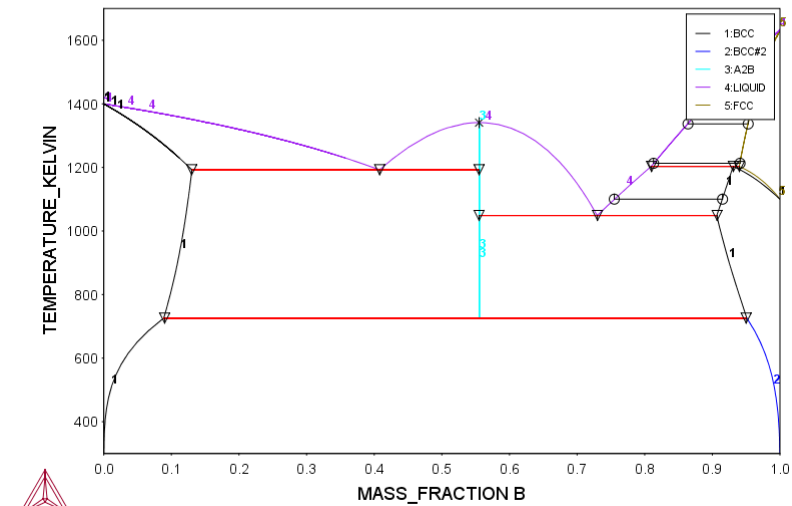
```



```

POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:Hit RETURN to continue
POST: @@ Add the experimental data
POST: a-e-d y exp36 0; 1
... the command in full is APPEND_EXPERIMENTAL_DATA
POST: plot
... the command in full is PLOT DIAGRAM
2016.05.16.14.20.34
A,B
P=1E5,N=1

```



```

POST:
POST:
POST:Hit RETURN to continue
POST: @@ Also calculate the enthalpies in the liquid
POST: ba
... the command in full is BACK
POLY_3: read,,,
... the command in full is READ_WORKSPACES
POLY_3:
POLY_3:
POLY_3: s-a-v 2 none
... the command in full is SET_AXIS_VARIABLE
POLY_3: s-c t=1773
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated          412 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution          0 s, total time          0 s
POLY_3: sh hmr
... the command in full is SHOW_VALUE
HMR=13116.476
POLY_3: l-st c

```

```

... the command in full is LIST_STATUS
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS      REF. STATE      T (K)          P (Pa)
A               ENTERED    SER
B               ENTERED    SER
POLY_3: s-r-s a liq * 1e5
... the command in full is SET_REFERENCE_STATE
POLY_3: s-r-s b liq * 1e5
... the command in full is SET_REFERENCE_STATE
POLY_3: save tcex36h y
... the command in full is SAVE_WORKSPACES
POLY_3: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 0.123400
...OK

Phase Region from 0.123400 for:
LIQUID
Global test at 3.23400E-01 .... OK
Global test at 5.73400E-01 .... OK
Global test at 8.23400E-01 .... OK
Global test at 9.53400E-01 .... OK
Global test at 1.00000E+00 .... OK
Terminating at 1.00000
Calculated 51 equilibria

Phase Region from 0.123400 for:
LIQUID
Global test at 8.34000E-02 .... OK
Global test at 3.34000E-02 .... OK
Terminating at 0.25000E-11
Calculated 28 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tce
x36h.POLY3
POLY_3: post

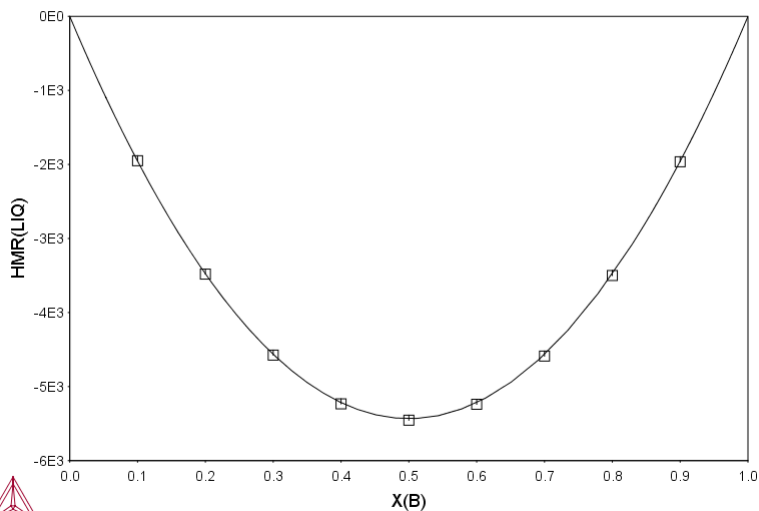
```

POLY-3 POSTPROCESSOR VERSION 3.2

```

POST: s-d-a x x(b)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y hmr(liq)
... the command in full is SET_DIAGRAM_AXIS
POST: a-e-d y exp36 0; 2
... the command in full is APPEND_EXPERIMENTAL_DATA
POST: plot
... the command in full is PLOT DIAGRAM
2016.05.16.14.20.35
A,B
P=1E5,N=1,T=1773

```



```

POST:
POST:Hit RETURN to continue
POST: @@ We can see the fitting results by the following method
POST: @@ Data points falling on the diagonal line indicates
POST: @@ perfect fitting.
POST: @@
POST: ba
... the command in full is BACK
POLY_3: ba
... the command in full is BACK

```

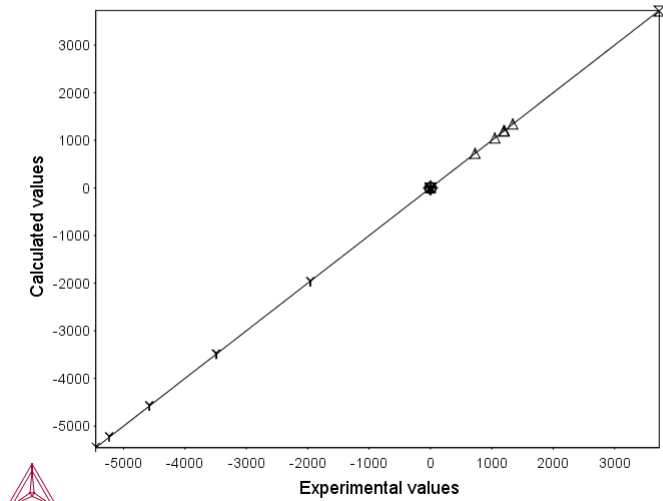
PARROT VERSION 5.3

```

Global minimization used as test only
PARROT: l-result gra pexp36 l,
... the command in full is LIST_RESULT
... the command in full is QUICK_EXPERIMENTAL_PLOT
... the command in full is PLOT_DIAGRAM

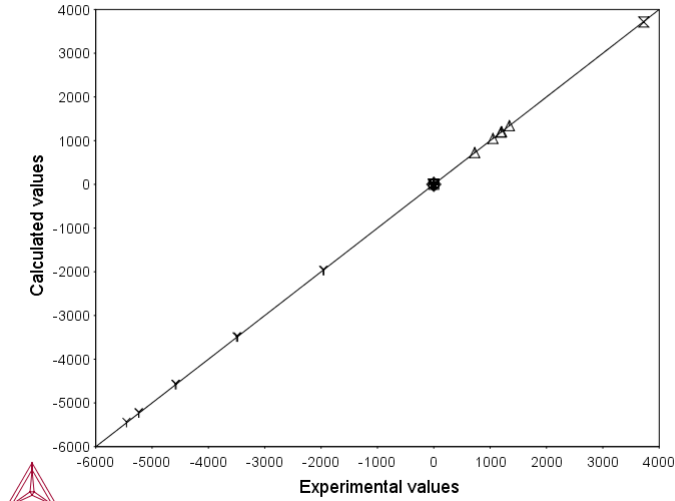
```

From PARROT optimization



POST: s-s-s y n -6000 4000  
... the command in full is SET\_SCALING\_STATUS  
POST: s-s-s x n -6000 4000  
... the command in full is SET\_SCALING\_STATUS  
POST: pl  
... the command in full is PLOT DIAGRAM

From PARROT optimization



POST: b  
... the command in full is BACK  
PARROT: set-inter  
... the command in full is SET\_INTERACTIVE  
PARROT: set-inter  
... the command in full is SET\_INTERACTIVE  
PARROT:

# tcex36a-tcex36b

```

PARROT>AboutMACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tcex36b.TCM"PARROT: s-s-f tcex36
... the command in full is SET_STORE_FILE
PARROT: @@ List parameters to be optimized, all zero initially
PARROT: l-a-v
... the command in full is LIST_ALL_VARIABLES
OUTPUT TO SCREEN OR FILE /SCREEN/:

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.  VALUE          START VALUE      SCALING FACTOR    REL.STAND.DEV
V1    2.03691169E+04   2.01820918E+04   2.01820918E+04   3.02498426E-02
V2    -2.94290453E+01  -2.90936108E+01  -2.90936108E+01  2.30117855E-02
V11   -2.17328114E+04  -2.18127452E+04  -2.18127452E+04  3.47139484E-02
V12    1.52102756E+01  1.55559572E+01  1.55559572E+01  5.38555420E-02
V15    2.42012673E+04  2.36701045E+04  2.36701045E+04  8.60926362E-02
V16   -8.38545778E+00  -7.56540324E+00  -7.56540324E+00  2.83695736E-01
V17    3.08774252E+03  3.00342248E+03  3.00342248E+03  2.37803227E-01
V19    2.20600539E+04  2.20133196E+04  2.20133196E+04  4.87694893E-01
V20   -7.07096129E+00  -6.72497818E+00  -6.72497818E+00  1.27666199E+00

NUMBER OF OPTIMIZING VARIABLES :    9
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM    5.15879918E-01 TO    6.73924422E-02
DEGREES OF FREEDOM    38. REDUCED SUM OF SQUARES    1.77348532E-03
PARROT: @@ Set alt mode to start
PARROT: s-alt Y
... the command in full is SET_ALTERNATE_MODE
PARROT: @@ Check if all equilibria can be calculated
PARROT: ed
... the command in full is EDIT_EXPERIMENTS
ED_EXP: read 1
... the command in full is READ_WORKSPACES
ED_EXP: c-a
... the command in full is COMPUTE_ALL_EQUILIBRIA
Eq  Lab  Iter Weight Temp  Exp  Fix phases or comments
1  AINV *alt*  1.0  1193.0    LIQUID A2B BCC
2  AINV *alt*  1.0  1341.0    LIQUID A2B
3  AINV *alt*  1.0  1049.0    LIQUID A2B BCC
4  AINV *alt*  1.0  1203.0    LIQUID BCC FCC
5  AINV *alt*  1.0  726.0     A2B BCC BCC#2
6  AINV *alt*  1.0  726.0     BCC BCC#2
Failed using alternate for FCC#1          setting weight to zero
10 ALF *alt*  1.0  1594.0    LIQUID FCC          setting weight to zero
Failed using alternate for FCC#1          setting weight to zero
11 ALF *alt*  1.0  1548.0    LIQUID FCC          setting weight to zero
Failed using alternate for FCC#1          setting weight to zero
12 ALF *alt*  1.0  1499.0    LIQUID FCC          setting weight to zero
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: @@ Equilibria with label ALF cannot use alt mode
ED_EXP: s-we 0 alf
... the command in full is SET_WEIGHT
Changed weight on          4 equilibria.
ED_EXP: c-a
... the command in full is COMPUTE_ALL_EQUILIBRIA
Eq  Lab  Iter Weight Temp  Exp  Fix phases or comments
118 AH      2  1.    1773.0    LIQUID
ED_EXP: save
... the command in full is SAVE_WORKSPACES
ED_EXP: @@ Save changes of weights before leaving editor
ED_EXP: ba
... the command in full is BACK
PARROT: @@ Optimize zero times as a check
PARROT: opt 0
... the command in full is OPTIMIZE_VARIABLES
Alternate calculation is on
Use    47 experiments, maximum is    2000
Use    1082 real workspace, maximum is    50000
PARROT: l-r C SCREEN
... the command in full is LIST_RESULT

=====
OUTPUT FROM  P A R R O T.  DATE 2016. 5.16   14:21:29

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS:    0

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00

```

RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04  
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)  
MAXFUN = 0 DMAX = 1.00000000E+02 H = 1.00000000E-04  
ACC = (INITIAL SUM OF SQUARES) \* 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.03691169E+04	2.01820918E+04	2.01820918E+04	3.02498426E-02
V2	-2.94290453E+01	-2.90936108E+01	-2.90936108E+01	2.30117855E-02
V11	-2.17328114E+04	-2.18127452E+04	-2.18127452E+04	3.47139484E-02
V12	1.52102756E+01	1.55559572E+01	1.55559572E+01	5.38555420E-02
V15	2.42012673E+04	2.36701045E+04	2.36701045E+04	8.60926362E-02
V16	-8.38545778E+00	-7.56540324E+00	-7.56540324E+00	2.83695736E-01
V17	3.08774252E+03	3.00342248E+03	3.00342248E+03	2.37803227E-01
V19	2.20600539E+04	2.20133196E+04	2.20133196E+04	4.87694893E-01
V20	-7.07096129E+00	-6.72497818E+00	-6.72497818E+00	1.27666199E+00

NUMBER OF OPTIMIZING VARIABLES : 9  
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO  
THE SUM OF SQUARES HAS CHANGED FROM 5.15879918E-01 TO 8.89279099E-02  
DEGREES OF FREEDOM 38. REDUCED SUM OF SQUARES 2.34020816E-03

Number of alternate equilibria 10

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS

DX=2E-2, P0=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%

HTR=HM(LIQUID)-HM(A2B)

1 Alternate equilibrium calc				0.00
2 Alternate equilibrium calc				0.19
2 HTR=3727	3714.	5.00E+02	-12.89	-2.5772E-02
3 Alternate equilibrium calc				0.00
4 Alternate equilibrium calc				0.00
5 Alternate equilibrium calc				0.01
6 Alternate equilibrium calc				0.01
20 Alternate equilibrium calc				0.01
21 Alternate equilibrium calc				0.00
22 Alternate equilibrium calc				0.01
23 Alternate equilibrium calc				0.00
100 ACR(B)=0.94	0.9397	2.85E-02	-2.7309E-04	-9.5946E-03
101 ACR(B)=0.84	0.8395	2.82E-02	-4.7482E-04	-1.6846E-02
102 ACR(B)=0.74	0.7408	2.81E-02	7.6893E-04	2.7408E-02
103 ACR(B)=0.64	0.6424	2.81E-02	2.4411E-03	8.6976E-02
104 ACR(B)=0.54	0.5435	2.82E-02	3.5079E-03	0.1243
105 ACR(B)=0.44	0.4429	2.85E-02	2.9003E-03	0.1016
106 ACR(B)=0.34	0.3395	2.90E-02	-5.0467E-04	-1.7386E-02
107 ACR(B)=0.23	0.2321	2.97E-02	2.0948E-03	7.0520E-02
108 ACR(B)=0.12	0.1194	3.06E-02	-5.9712E-04	-1.9513E-02
110 HMR(LIQUID)=-1964	-1956.	5.00E+02	8.047	1.6094E-02
111 HMR(LIQUID)=-3500	-3477.	5.00E+02	22.75	4.5500E-02
112 HMR(LIQUID)=-4588	-4564.	5.00E+02	24.11	4.8219E-02
113 HMR(LIQUID)=-5239	-5216.	5.00E+02	23.13	4.6251E-02
114 HMR(LIQUID)=-5454	-5433.	5.00E+02	20.80	4.1594E-02
115 HMR(LIQUID)=-5233	-5216.	5.00E+02	17.13	3.4251E-02
116 HMR(LIQUID)=-4575	-4564.	5.00E+02	11.11	2.2219E-02
117 HMR(LIQUID)=-3481	-3477.	5.00E+02	3.750	7.5004E-03
118 HMR(LIQUID)=-1950	-1956.	5.00E+02	-5.953	-1.1906E-02

PARROT:

PARROT:Hit RETURN to continue

PARROT: @@ Note only one error from alternate calculations. This error represents

PARROT: @@ the difference in chemical potentials of the phases.

PARROT: @@ Experiments with just one phase is calculated as normal.

PARROT: @@ Next command supresses listing of parameters.

PARROT: s-o-l 1 Y Y N n N

... the command in full is SET\_OUTPUT\_LEVELS

PARROT: l-r C SCREEN

... the command in full is LIST\_RESULT

=====

OUTPUT FROM P A R R O T. DATE 2016. 5.16 14:21:29

\*\*\* SUCCESSFUL OPTIMIZATION. \*\*\*  
NUMBER OF ITERATIONS: 0

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N  
MINIMUM SAVE ON FILE: Y  
ERROR FOR INEQUALITIES = 1.00000000E+00  
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04  
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)  
MAXFUN = 0 DMAX = 1.00000000E+02 H = 1.00000000E-04  
ACC = (INITIAL SUM OF SQUARES) \* 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.03691169E+04	2.01820918E+04	2.01820918E+04	3.02498426E-02
V2	-2.94290453E+01	-2.90936108E+01	-2.90936108E+01	2.30117855E-02
V11	-2.17328114E+04	-2.18127452E+04	-2.18127452E+04	3.47139484E-02
V12	1.52102756E+01	1.55559572E+01	1.55559572E+01	5.38555420E-02
V15	2.42012673E+04	2.36701045E+04	2.36701045E+04	8.60926362E-02
V16	-8.38545778E+00	-7.56540324E+00	-7.56540324E+00	2.83695736E-01
V17	3.08774252E+03	3.00342248E+03	3.00342248E+03	2.37803227E-01



V19 2.20600539E+04 2.20133196E+04 2.20133196E+04 4.87694893E-01  
V20 -7.07096129E+00 -6.72497818E+00 -6.72497818E+00 1.27666199E+00

NUMBER OF OPTIMIZING VARIABLES : 9  
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO  
THE SUM OF SQUARES HAS CHANGED FROM 5.15879918E-01 TO 8.89279099E-02  
DEGREES OF FREEDOM 38. REDUCED SUM OF SQUARES 2.34020816E-03

Number of alternate equilibria 10

SYMBOL	STATUS	VALUE/FUNCTION
1 R	80000000	8.3145100E+00
2 RTLNP	20000000	+R*T*LN(1E-05*P)
3 V1	48000000	2.0369117E+04
4 V2	48000000	-2.9429045E+01
13 V11	48000000	-2.1732811E+04
14 V12	48000000	1.5210276E+01
17 V15	48000000	2.4201267E+04
18 V16	48000000	-8.3854578E+00
19 V17	48000000	3.0877425E+03
21 V19	48000000	2.2060054E+04
22 V20	48000000	-7.0709613E+00

LIQUID  
EXCESS MODEL IS REDLICH-KISTER\_MUGGIANU  
CONSTITUENTS: A,B

G(LIQUID,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +14000-10\*T  
G(LIQUID,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +18000-12\*T  
L(LIQUID,A,B;0) = 500.00<T< 2000.00: +V11+V12\*T  
L(LIQUID,A,B;1) = 500.00<T< 2000.00: +V13+V14\*T

A2B  
2 SUBLATTICES, SITES 2: 1  
CONSTITUENTS: A : B

G(A2B,A;B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =  
500.00<T< 2000.00: +V1+V2\*T+V3\*T\*LN(T)

BCC  
EXCESS MODEL IS REDLICH-KISTER\_MUGGIANU  
CONSTITUENTS: A,B

G(BCC,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +0.0  
G(BCC,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +0.0  
L(BCC,A,B;0) = 500.00<T< 2000.00: +V15+V16\*T  
L(BCC,A,B;1) = 500.00<T< 2000.00: +V17+V18\*T

FCC  
EXCESS MODEL IS REDLICH-KISTER\_MUGGIANU  
CONSTITUENTS: A,B

G(FCC,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +408  
G(FCC,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +3300-3\*T  
L(FCC,A,B;0) = 500.00<T< 2000.00: +V19+V20\*T  
L(FCC,A,B;1) = 500.00<T< 2000.00: +V21+V22\*T

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS

DX=2E-2, P0=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%

HTR=HM(LIQUID)-HM(A2B)

1 Alternate equilibrium calc				0.00
2 Alternate equilibrium calc				0.19
2 HTR=3727	3714.	5.00E+02	-12.89	-2.5772E-02
3 Alternate equilibrium calc				0.00
4 Alternate equilibrium calc				0.00
5 Alternate equilibrium calc				0.01
6 Alternate equilibrium calc				0.01
20 Alternate equilibrium calc				0.01
21 Alternate equilibrium calc				0.00
22 Alternate equilibrium calc				0.01
23 Alternate equilibrium calc				0.00
100 ACR(B)=0.94	0.9397	2.85E-02	-2.7309E-04	-9.5946E-03
101 ACR(B)=0.84	0.8395	2.82E-02	-4.7482E-04	-1.6846E-02
102 ACR(B)=0.74	0.7408	2.81E-02	7.6893E-04	2.7408E-02
103 ACR(B)=0.64	0.6424	2.81E-02	2.4411E-03	8.6976E-02
104 ACR(B)=0.54	0.5435	2.82E-02	3.5079E-03	0.1243
105 ACR(B)=0.44	0.4429	2.85E-02	2.9003E-03	0.1016
106 ACR(B)=0.34	0.3395	2.90E-02	-5.0467E-04	-1.7386E-02
107 ACR(B)=0.23	0.2321	2.97E-02	2.0948E-03	7.0520E-02
108 ACR(B)=0.12	0.1194	3.06E-02	-5.9712E-04	-1.9513E-02
110 HMR(LIQUID)=-1964	-1956.	5.00E+02	8.047	1.6094E-02
111 HMR(LIQUID)=-3500	-3477.	5.00E+02	22.75	4.5500E-02
112 HMR(LIQUID)=-4588	-4564.	5.00E+02	24.11	4.8219E-02
113 HMR(LIQUID)=-5239	-5216.	5.00E+02	23.13	4.6251E-02
114 HMR(LIQUID)=-5454	-5433.	5.00E+02	20.80	4.1594E-02
115 HMR(LIQUID)=-5233	-5216.	5.00E+02	17.13	3.4251E-02
116 HMR(LIQUID)=-4575	-4564.	5.00E+02	11.11	2.2219E-02
117 HMR(LIQUID)=-3481	-3477.	5.00E+02	3.750	7.5004E-03
118 HMR(LIQUID)=-1950	-1956.	5.00E+02	-5.953	-1.1906E-02

PARROT:

PARROT: @@ Now optimize

PARROT: opt 30

... the command in full is OPTIMIZE\_VARIABLES

Alternate calculation is on

Use 47 experiments, maximum is 2000

Use 1082 real workspace, maximum is 50000

The following output is provided by subroutine VA05A

AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 8.89279099E-02  
1 1.0093E+00 2 1.0115E+00 3 9.9634E-01 4 9.7778E-01 5 1.0224E+00  
6 1.1084E+00 7 1.0281E+00 8 1.0021E+00 9 1.0514E+00

AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 8.89950288E-02

```

1 1.0094E+00 2 1.0115E+00 3 9.9634E-01 4 9.7778E-01 5 1.0224E+00
6 1.1084E+00 7 1.0281E+00 8 1.0021E+00 9 1.0514E+00

AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 8.89370493E-02
1 1.0093E+00 2 1.0115E+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 3 RD ITERATION WE HAVE THE SUM OF SQUARES 8.79489886E-02
1 1.0093E+00 2 1.0115E+00 3 9.9644E-01 4 9.7778E-01 5 1.0224E+00
6 1.1084E+00 7 1.0281E+00 8 1.0021E+00 9 1.0514E+00

AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 8.85893317E-02
1 1.0093E+00 2 1.0115E+00 3 9.9644E-01 4 9.7788E-01 5 1.0224E+00
6 1.1084E+00 7 1.0281E+00 8 1.0021E+00 9 1.0514E+00

AT THE 5 TH ITERATION WE HAVE THE SUM OF SQUARES 8.79262642E-02
1 1.0093E+00 2 1.0115E+00 3 9.9644E-01 4 9.7778E-01 5 1.0225E+00
6 1.1084E+00 7 1.0281E+00 8 1.0021E+00 9 1.0514E+00

AT THE 6 TH ITERATION WE HAVE THE SUM OF SQUARES 8.79317664E-02
1 1.0093E+00 2 1.0115E+00 3 9.9644E-01 4 9.7778E-01 5 1.0225E+00
6 1.1085E+00 7 1.0281E+00 8 1.0021E+00 9 1.0514E+00

AT THE 7 TH ITERATION WE HAVE THE SUM OF SQUARES 8.79245152E-02
1 1.0093E+00 2 1.0115E+00 3 9.9644E-01 4 9.7778E-01 5 1.0225E+00
6 1.1084E+00 7 1.0282E+00 8 1.0021E+00 9 1.0514E+00

AT THE 8 TH ITERATION WE HAVE THE SUM OF SQUARES 8.79198012E-02
1 1.0093E+00 2 1.0115E+00 3 9.9644E-01 4 9.7778E-01 5 1.0225E+00
6 1.1084E+00 7 1.0282E+00 8 1.0022E+00 9 1.0514E+00

AT THE 9 TH ITERATION WE HAVE THE SUM OF SQUARES 8.79216928E-02
1 1.0093E+00 2 1.0115E+00 3 9.9644E-01 4 9.7778E-01 5 1.0225E+00
6 1.1084E+00 7 1.0282E+00 8 1.0022E+00 9 1.0515E+00

AT THE 10 TH ITERATION WE HAVE THE SUM OF SQUARES 6.30012576E-02
1 1.0090E+00 2 1.0115E+00 3 1.0000E+00 4 9.7542E-01 5 1.0226E+00
6 1.1084E+00 7 1.0282E+00 8 1.0022E+00 9 1.0514E+00

AT THE 11 TH ITERATION WE HAVE THE SUM OF SQUARES 6.00250613E-02
1 1.0062E+00 2 1.0109E+00 3 9.9912E-01 4 9.7423E-01 5 1.0235E+00
6 1.1105E+00 7 1.0290E+00 8 1.0016E+00 9 1.0501E+00

AT THE 12 TH ITERATION WE HAVE THE SUM OF SQUARES 5.93161822E-02
1 1.0057E+00 2 1.0092E+00 3 9.9970E-01 4 9.7424E-01 5 1.0255E+00
6 1.1178E+00 7 1.0318E+00 8 1.0004E+00 9 1.0481E+00

AT THE 13 TH ITERATION WE HAVE THE SUM OF SQUARES 5.88760571E-02
1 1.0049E+00 2 1.0059E+00 3 9.9988E-01 4 9.7463E-01 5 1.0295E+00
6 1.1320E+00 7 1.0370E+00 8 9.9745E-01 9 1.0425E+00

THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 13 iterations
1 1.0049E+00 2 1.0059E+00 3 9.9988E-01 4 9.7463E-01 5 1.0295E+00
6 1.1320E+00 7 1.0370E+00 8 9.9745E-01 9 1.0425E+00

1 6.9039E-03 2 6.9039E-03 3 1.5738E-03 4 2.6800E-03 5 1.3310E-01
6 -1.3983E-01 7 -1.4164E-03 8 7.6472E-03 9 7.6472E-03 10 -1.0561E-04
11 3.2960E-03 12 2.1369E-03 13 2.5829E-04 14 3.0760E-03 15 6.0633E-04
16 1.2976E-03 17 1.2976E-03 18 2.3664E-05 19 1.6822E-03 20 2.3664E-05
21 1.6822E-03 22 -2.0443E-03 23 1.7694E-03 24 3.4709E-03 25 3.3350E-04
26 -2.5368E-03 27 3.2555E-03 28 -1.4427E-03 29 3.8328E-03 30 -1.3478E-02
31 -3.0855E-02 32 -6.3336E-04 33 4.3684E-02 34 6.7408E-02 35 3.5765E-02
36 -8.4872E-02 37 1.1726E-02 38 -5.6892E-02 39 2.1632E-03 40 2.0734E-02
41 1.5714E-02 42 9.1017E-03 43 2.8977E-03 44 -2.8983E-03 45 -1.0286E-02
46 -1.7266E-02 47 -2.5837E-02

```

THE SUM OF SQUARES IS 5.88760571E-02

PARROT: cont 30

... the command in full is CONTINUE\_OPTIMIZATION

It is safe to CONTINUE only after TOO MANY ITERATIONS  
and no change in variables and experiments ...  
Now anything can happen ...

PARROT: l-r C SCREEN

... the command in full is LIST\_RESULT

-----  
OUTPUT FROM P A R R O T. DATE 2016. 5.16 14:21:29

\*\*\* SUCCESSFUL OPTIMIZATION. \*\*\*  
NUMBER OF ITERATIONS: 14

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N  
MINIMUM SAVE ON FILE: Y  
ERROR FOR INEQUALITIES = 1.00000000E+00  
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04  
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)  
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04  
ACC = (INITIAL SUM OF SQUARES) \* 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.02809885E+04	2.01820918E+04	2.01820918E+04	7.95747010E-02
V2	-2.92651699E+01	-2.90936108E+01	-2.90936108E+01	3.44415373E-01
V11	-2.18102047E+04	-2.18127452E+04	-2.18127452E+04	3.96943915E-02
V12	1.51613087E+01	1.55559572E+01	1.55559572E+01	5.70071432E-02
V15	2.43675665E+04	2.36701045E+04	2.36701045E+04	6.28240698E-01
V16	-8.56377518E+00	-7.56540324E+00	-7.56540324E+00	2.32375383E+00
V17	3.11464876E+03	3.00342248E+03	3.00342248E+03	1.51251851E+00
V19	2.19570764E+04	2.20133196E+04	2.20133196E+04	4.62338048E+00
V20	-7.01093190E+00	-6.72497818E+00	-6.72497818E+00	1.17285936E+01

NUMBER OF OPTIMIZING VARIABLES : 9  
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO  
THE SUM OF SQUARES HAS CHANGED FROM 8.89279099E-02 TO 5.88760571E-02  
DEGREES OF FREEDOM 38. REDUCED SUM OF SQUARES 1.54936992E-03

Number of alternate equilibria 10

SYMBOL	STATUS	VALUE/FUNCTION
1 R	80000000	8.3145100E+00
2 RTLNP	20000000	+R*T*LN(1E-05*P)
3 V1	48000000	2.0280989E+04
4 V2	48000000	-2.9265170E+01
13 V11	48000000	-2.1810205E+04
14 V12	48000000	1.5161309E+01
17 V15	48000000	2.4367567E+04
18 V16	48000000	-8.5637752E+00
19 V17	48000000	3.1146488E+03
21 V19	48000000	2.1957076E+04
22 V20	48000000	-7.0109319E+00

LIQUID  
EXCESS MODEL IS REDLICH-KISTER\_MUGGIANU  
CONSTITUENTS: A,B

G(LIQUID,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +14000-10\*T  
G(LIQUID,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +18000-12\*T  
L(LIQUID,A,B;0) = 500.00<T< 2000.00: +V11+V12\*T  
L(LIQUID,A,B;1) = 500.00<T< 2000.00: +V13+V14\*T

A2B  
2 SUBLATTICES, SITES 2: 1  
CONSTITUENTS: A : B

G(A2B,A;B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =  
500.00<T< 2000.00: +V1+V2\*T+V3\*T\*LN(T)

BCC  
EXCESS MODEL IS REDLICH-KISTER\_MUGGIANU  
CONSTITUENTS: A,B

G(BCC,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +0.0  
G(BCC,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +0.0  
L(BCC,A,B;0) = 500.00<T< 2000.00: +V15+V16\*T  
L(BCC,A,B;1) = 500.00<T< 2000.00: +V17+V18\*T

FCC  
EXCESS MODEL IS REDLICH-KISTER\_MUGGIANU  
CONSTITUENTS: A,B

G(FCC,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +408  
G(FCC,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +3300-3\*T  
L(FCC,A,B;0) = 500.00<T< 2000.00: +V19+V20\*T  
L(FCC,A,B;1) = 500.00<T< 2000.00: +V21+V22\*T

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS

DX=2E-2, P0=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%

HTR=HM(LIQUID)-HM(A2B)

1 Alternate equilibrium calc				0.01
2 Alternate equilibrium calc				0.19
2 HTR=3727	3726.	5.00E+02	-0.7082	-1.4164E-03
3 Alternate equilibrium calc				0.01
4 Alternate equilibrium calc				0.00
5 Alternate equilibrium calc				0.00
6 Alternate equilibrium calc				0.00
20 Alternate equilibrium calc				0.00
21 Alternate equilibrium calc				0.00
22 Alternate equilibrium calc				0.00
23 Alternate equilibrium calc				0.00
100 ACR(B)=0.94	0.9396	2.85E-02	-3.8404E-04	-1.3478E-02
101 ACR(B)=0.84	0.8391	2.82E-02	-8.7121E-04	-3.0855E-02
102 ACR(B)=0.74	0.7400	2.81E-02	-1.7806E-05	-6.3336E-04
103 ACR(B)=0.64	0.6412	2.81E-02	1.2286E-03	4.3684E-02
104 ACR(B)=0.54	0.5419	2.83E-02	1.9060E-03	6.7408E-02
105 ACR(B)=0.44	0.4410	2.86E-02	1.0218E-03	3.5765E-02
106 ACR(B)=0.34	0.3375	2.90E-02	-2.4631E-03	-8.4872E-02
107 ACR(B)=0.23	0.2303	2.96E-02	3.4765E-04	1.1726E-02
108 ACR(B)=0.12	0.1183	3.05E-02	-1.7336E-03	-5.6892E-02
110 HMR(LIQUID)=-1964	-1963.	5.00E+02	1.082	2.1632E-03
111 HMR(LIQUID)=-3500	-3490.	5.00E+02	10.37	2.0734E-02
112 HMR(LIQUID)=-4588	-4580.	5.00E+02	7.857	1.5714E-02
113 HMR(LIQUID)=-5239	-5234.	5.00E+02	4.551	9.1017E-03
114 HMR(LIQUID)=-5454	-5453.	5.00E+02	1.449	2.8977E-03
115 HMR(LIQUID)=-5233	-5234.	5.00E+02	-1.449	-2.8983E-03
116 HMR(LIQUID)=-4575	-4580.	5.00E+02	-5.143	-1.0286E-02
117 HMR(LIQUID)=-3481	-3490.	5.00E+02	-8.633	-1.7266E-02
118 HMR(LIQUID)=-1950	-1963.	5.00E+02	-12.92	-2.5837E-02

PARROT:

PARROT:Hit RETURN to continue

PARROT: @@ The liquid data fitted reasonable, fix its parameters to simplify

PARROT: l-p-d liq

... the command in full is LIST\_PHASE\_DATA

LIQUID  
EXCESS MODEL IS REDLICH-KISTER\_MUGGIANU  
CONSTITUENTS: A,B

G(LIQUID,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +14000-10\*T  
G(LIQUID,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +18000-12\*T  
L(LIQUID,A,B;0) = 500.00<T< 2000.00: +V11+V12\*T  
L(LIQUID,A,B;1) = 500.00<T< 2000.00: +V13+V14\*T

PARROT: s-f-v 11-14

... the command in full is SET\_FIX\_VARIABLE

PARROT: @@ Rescale the start values of the parameters to current values

```

PARROT: resc
... the command in full is RESCALE_VARIABLES
PARROT: l-a-v
... the command in full is LIST_ALL_VARIABLES
OUTPUT TO SCREEN OR FILE /SCREEN/:-

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.  VALUE          START VALUE    SCALING FACTOR    REL.STAND.DEV
V1    2.02809885E+04    2.02809885E+04    2.02809885E+04    0.00000000E+00
V2    -2.92651699E+01   -2.92651699E+01   -2.92651699E+01   0.00000000E+00
V11   -2.18102047E+04    2.43675665E+04    2.43675665E+04    0.00000000E+00
V12    1.51613087E+01    2.43675665E+04    2.43675665E+04    0.00000000E+00
V15    2.43675665E+04    2.43675665E+04    2.43675665E+04    0.00000000E+00
V16   -8.56377518E+00   -8.56377518E+00   -8.56377518E+00   0.00000000E+00
V17    3.11464876E+03    3.11464876E+03    3.11464876E+03    0.00000000E+00
V19    2.19570764E+04    2.19570764E+04    2.19570764E+04    0.00000000E+00
V20   -7.01093190E+00   -7.01093190E+00   -7.01093190E+00   0.00000000E+00

NUMBER OF OPTIMIZING VARIABLES : 7
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
PARROT:Hit RETURN to continue
PARROT: mac tcex36cpd
... the command in full is MACRO_FILE_OPEN
PARROT: set-echo
NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
... the command in full is GOTO_MODULE
POLY_3:
POLY_3: @@ In PARROT, the global minimization is turned off automatically.
POLY_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY_3: @@ message will be given.
POLY_3:
POLY_3: advanced-option global yes,,
... the command in full is ADVANCED_OPTIONS
Settings for global minimization:
*** WARNING *** Global equilibrium calculation may create new composition sets
and this may corrupt your PARROT work file (.PAR file).
Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY_3:
POLY_3: def-com,,,,
... the command in full is DEFINE_COMPONENTS
POLY_3: s-a-v 1 w(b) 0 1,,,,
... the command in full is SET_AXIS_VARIABLE
The condition W(B)=.1234 created
POLY_3: s-a-v 2 t 300 1700,,,,
... the command in full is SET_AXIS_VARIABLE
The condition T=942.2 created
POLY_3: s-c t=500
... the command in full is SET_CONDITION
POLY_3: l-c
... the command in full is LIST_CONDITIONS
W(B)=0.1234, P=1E5, N=1, T=500
DEGREES OF FREEDOM 0
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 412 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY_3: save tcex36 y
... the command in full is SAVE_WORKSPACES

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

POLY_3: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23

```

```

Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

Phase region boundary 1 at: 7.140E-01 3.100E+02
  BCC
  ** BCC#2
  Calculated.. 2 equilibria
  Terminating at axis limit.

Phase region boundary 2 at: 7.141E-01 3.000E+02
  BCC
  ** BCC#2
  Calculated. 14 equilibria

Phase region boundary 3 at: 6.817E-01 7.266E+02
  ** A2B
  BCC
  ** BCC#2

Phase region boundary 4 at: 3.625E-01 7.266E+02
  ** A2B
  BCC
  Calculated. 15 equilibria

Phase region boundary 5 at: 3.778E-01 1.185E+03
  ** LIQUID
  ** A2B
  BCC

Phase region boundary 6 at: 2.888E-01 1.185E+03
  ** LIQUID
  BCC
  Calculated 28 equilibria

Phase region boundary 7 at: 4.900E-01 1.185E+03
  ** LIQUID
  A2B
  Calculated. 33 equilibria

Phase region boundary 8 at: 6.482E-01 1.039E+03
  ** LIQUID
  A2B
  ** BCC

Phase region boundary 9 at: 7.637E-01 1.039E+03
  A2B
  ** BCC
  Calculated. 10 equilibria
  Terminating at known equilibrium

Phase region boundary 10 at: 8.259E-01 1.039E+03
  LIQUID
  ** BCC
  Calculated. 8 equilibria

Phase region boundary 11 at: 8.759E-01 1.204E+03
  LIQUID
  ** BCC
  ** FCC

Phase region boundary 12 at: 8.811E-01 1.204E+03
  LIQUID
  ** FCC
  Calculated 32 equilibria

Phase region boundary 13 at: 9.361E-01 1.204E+03
  BCC
  ** FCC
  Calculated 20 equilibria

Phase region boundary 14 at: 7.140E-01 3.100E+02
  BCC
  ** BCC#2
  Calculated. 13 equilibria
  Terminating at known equilibrium

Phase region boundary 15 at: 7.140E-01 3.100E+02
  BCC
  ** BCC#2
  Calculated.. 2 equilibria
  Terminating at known equilibrium
  Terminating at axis limit.

Phase region boundary 16 at: 7.140E-01 3.100E+02
  BCC
  ** BCC#2
  Calculated. 13 equilibria
  Terminating at known equilibrium

Phase region boundary 17 at: 7.140E-01 3.100E+02
  BCC
  ** BCC#2
  Calculated.. 2 equilibria
  Terminating at known equilibrium
  Terminating at axis limit.

Phase region boundary 18 at: 7.140E-01 3.100E+02
  BCC
  ** BCC#2
  Calculated. 13 equilibria
  Terminating at known equilibrium

Phase region boundary 19 at: 7.140E-01 3.100E+02
  BCC
  ** BCC#2
  Calculated.. 2 equilibria
  Terminating at known equilibrium
  Terminating at axis limit.

Phase region boundary 20 at: 7.140E-01 3.100E+02
  BCC
  ** BCC#2
  Calculated. 13 equilibria

```

Terminating at known equilibrium

Phase region boundary 21 at: 7.140E-01 3.100E+02  
\*\* BCC  
BCC#2  
Calculated.. 2 equilibria  
Terminating at known equilibrium  
Terminating at axis limit.

Phase region boundary 22 at: 7.140E-01 3.100E+02  
\*\* BCC  
BCC#2  
Calculated. 13 equilibria  
Terminating at known equilibrium

Phase region boundary 23 at: 7.140E-01 3.100E+02  
\*\* BCC  
BCC#2  
Calculated.. 2 equilibria  
Terminating at known equilibrium  
Terminating at axis limit.

Phase region boundary 24 at: 7.140E-01 3.100E+02  
\*\* BCC  
BCC#2  
Calculated. 13 equilibria  
Terminating at known equilibrium

Phase region boundary 25 at: 3.646E-01 7.700E+02  
\*\* A2B  
BCC  
Calculated 10 equilibria

Phase region boundary 26 at: 3.646E-01 7.700E+02  
\*\* A2B  
BCC  
Calculated. 3 equilibria  
Terminating at known equilibrium

Phase region boundary 27 at: 3.646E-01 7.700E+02  
\*\* A2B  
BCC  
Calculated. 13 equilibria  
Terminating at known equilibrium

Phase region boundary 28 at: 7.909E-01 7.700E+02  
\*\* A2B  
BCC  
Calculated 10 equilibria

Phase region boundary 29 at: 7.909E-01 7.700E+02  
\*\* A2B  
BCC  
Calculated. 3 equilibria  
Terminating at known equilibrium

Phase region boundary 30 at: 7.909E-01 7.700E+02  
\*\* A2B  
BCC  
Calculated. 9 equilibria  
Terminating at known equilibrium

Phase region boundary 31 at: 2.435E-01 1.230E+03  
\*\* LIQUID  
BCC  
Calculated. 4 equilibria  
Terminating at known equilibrium

Phase region boundary 32 at: 2.435E-01 1.230E+03  
\*\* LIQUID  
BCC  
Calculated 26 equilibria

Phase region boundary 33 at: 8.867E-01 1.230E+03  
\*\* LIQUID  
FCC  
Calculated. 2 equilibria  
Terminating at known equilibrium

Phase region boundary 34 at: 8.867E-01 1.230E+03  
\*\* LIQUID  
FCC  
Calculated 29 equilibria

Phase region boundary 35 at: 6.404E-03 1.397E+03  
LIQUID  
\*\* BCC  
Calculated 10 equilibria

Phase region boundary 36 at: 6.404E-03 1.397E+03  
LIQUID  
\*\* BCC  
Calculated. 13 equilibria  
Terminating at known equilibrium

Phase region boundary 37 at: 2.295E-01 1.243E+03  
LIQUID  
\*\* BCC  
Calculated 22 equilibria

Phase region boundary 38 at: 2.295E-01 1.243E+03  
LIQUID  
\*\* BCC  
Calculated. 4 equilibria  
Terminating at known equilibrium

Phase region boundary 39 at: 6.122E-01 1.215E+03  
LIQUID  
\*\* A2B  
Calculated. 12 equilibria  
Terminating at known equilibrium

Phase region boundary 40 at: 6.122E-01 1.215E+03  
LIQUID  
\*\* A2B  
Calculated. 8 equilibria

Terminating at known equilibrium

Phase region boundary 41 at: 9.927E-01 1.613E+03  
LIQUID

\*\* FCC  
Calculated. 19 equilibria  
Terminating at known equilibrium

Phase region boundary 42 at: 9.927E-01 1.613E+03  
LIQUID

\*\* FCC  
Calculated 13 equilibria  
\*\*\* BUFFER SAVED ON FILE:

c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tce  
x36.POLY3  
CPU time for mapping 1 seconds

POLY\_3: post

POST: s-l d

... the command in full is SET\_LABEL\_CURVE\_OPTION

POST: plot

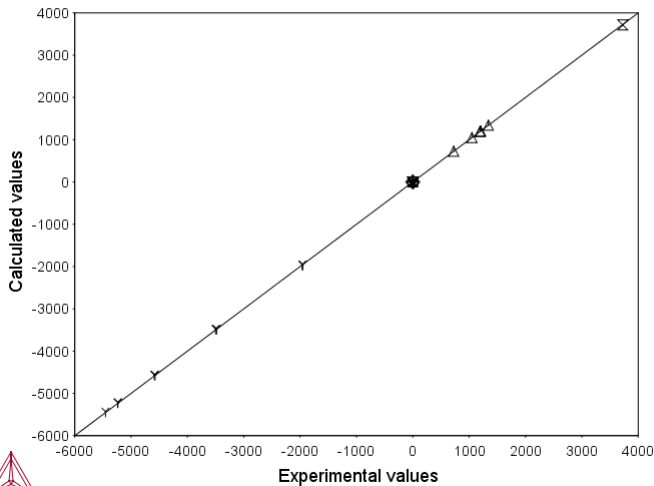
... the command in full is PLOT DIAGRAM

From PARROT optimization

2016.05.16.14.21.34

A,B

P=1E5,N=1



△ 1: T  
□ 2: W(LIQUID)  
◇ 3: W(BCC,B)  
⊗ 4: HTR  
▽ 5: W(LIQUID)  
+ 6: W(BCC,A)  
\* 7: W(FCC,A)  
× 8: X(BCC,B)  
⊙ 9: X(BCC#2)  
★ 10: ACR(B)  
γ 11: HMR(LIQUID)  
⊗ 12:  
⊗ 13:  
\* 14:  
+ 15:  
⊙ 16: DGM  
⊗ 17: inequality  
■ 20: others

POST:

POST: set-inter

... the command in full is SET\_INTERACTIVE\_MODE

POST:Hit RETURN to continue

POST: ba

... the command in full is BACK

POLY\_3: ba

... the command in full is BACK

PARROT VERSION 5.3

Global minimization used as test only

PARROT: @@ This does not look very good, optimize more ...

PARROT: opt 30

... the command in full is OPTIMIZE\_VARIABLES

Alternate calculation is on

Use 47 experiments, maximum is 2000

Use 824 real workspace, maximum is 50000

The following output is provided by subroutine VA05A

```
AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 5.88760571E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00

AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 5.88814903E-02
1 1.0001E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00

AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 5.88785935E-02
1 1.0000E+00 2 1.0001E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00

AT THE 3 RD ITERATION WE HAVE THE SUM OF SQUARES 5.88751225E-02
1 1.0000E+00 2 1.0000E+00 3 1.0001E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00

AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 5.88749460E-02
1 1.0000E+00 2 1.0000E+00 3 1.0001E+00 4 1.0001E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00

AT THE 5 TH ITERATION WE HAVE THE SUM OF SQUARES 5.88746800E-02
1 1.0000E+00 2 1.0000E+00 3 1.0001E+00 4 1.0001E+00 5 1.0001E+00
6 1.0000E+00 7 1.0000E+00

AT THE 6 TH ITERATION WE HAVE THE SUM OF SQUARES 5.88754522E-02
1 1.0000E+00 2 1.0000E+00 3 1.0001E+00 4 1.0001E+00 5 1.0001E+00
6 1.0001E+00 7 1.0000E+00

AT THE 7 TH ITERATION WE HAVE THE SUM OF SQUARES 5.88744378E-02
1 1.0000E+00 2 1.0000E+00 3 1.0001E+00 4 1.0001E+00 5 1.0001E+00
6 1.0000E+00 7 1.0001E+00

THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 7 iterations
1 1.0000E+00 2 1.0000E+00 3 1.0001E+00 4 1.0001E+00 5 1.0001E+00
6 1.0000E+00 7 1.0001E+00

1 6.9039E-03 2 6.9039E-03 3 1.5746E-03 4 2.8286E-03 5 1.3310E-01
6 -1.3983E-01 7 -1.4164E-03 8 7.6472E-03 9 7.6472E-03 10 1.9847E-06
11 3.3001E-03 12 2.2286E-03 13 2.5992E-04 14 3.0133E-03 15 6.0473E-04
16 1.1906E-03 17 1.1906E-03 18 2.3705E-04 19 1.3648E-03 20 2.3705E-04
```

```
21 1.3648E-03 22 -2.1141E-03 23 1.7687E-03 24 3.4041E-03 25 3.3248E-04
26 -2.5998E-03 27 3.2539E-03 28 -1.3406E-03 29 3.8359E-03 30 -1.3478E-02
31 -3.0855E-02 32 -6.3336E-04 33 4.3684E-02 34 6.7408E-02 35 3.5765E-02
36 -8.4872E-02 37 1.1726E-02 38 -5.6892E-02 39 2.1632E-03 40 2.0734E-02
41 1.5714E-02 42 9.1017E-03 43 2.8977E-03 44 -2.8983E-03 45 -1.0286E-02
46 -1.7266E-02 47 -2.5837E-02
```

THE SUM OF SQUARES IS 5.88744378E-02

PARROT: resc

... the command in full is RESCALE\_VARIABLES

PARROT: opt 30

... the command in full is OPTIMIZE\_VARIABLES

Alternate calculation is on

Use 47 experiments, maximum is 2000

Use 824 real workspace, maximum is 50000

The following output is provided by subroutine VA05A

```
AT THE 0 TH ITERATION WE HAVE THE SUM OF SQUARES 5.88744378E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00
```

```
AT THE 1 ST ITERATION WE HAVE THE SUM OF SQUARES 5.88798231E-02
1 1.0001E+00 2 1.0000E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00
```

```
AT THE 2 ND ITERATION WE HAVE THE SUM OF SQUARES 5.88770243E-02
1 1.0000E+00 2 1.0001E+00 3 1.0000E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00
```

```
AT THE 3 RD ITERATION WE HAVE THE SUM OF SQUARES 5.88744664E-02
1 1.0000E+00 2 1.0000E+00 3 1.0001E+00 4 1.0000E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00
```

```
AT THE 4 TH ITERATION WE HAVE THE SUM OF SQUARES 5.88743603E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0001E+00 5 1.0000E+00
6 1.0000E+00 7 1.0000E+00
```

```
AT THE 5 TH ITERATION WE HAVE THE SUM OF SQUARES 5.88740934E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0001E+00 5 1.0001E+00
6 1.0000E+00 7 1.0000E+00
```

```
AT THE 6 TH ITERATION WE HAVE THE SUM OF SQUARES 5.88747821E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0001E+00 5 1.0001E+00
6 1.0001E+00 7 1.0000E+00
```

```
AT THE 7 TH ITERATION WE HAVE THE SUM OF SQUARES 5.88738857E-02
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0001E+00 5 1.0001E+00
6 1.0000E+00 7 1.0001E+00
```

```
THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED 7 iterations
1 1.0000E+00 2 1.0000E+00 3 1.0000E+00 4 1.0001E+00 5 1.0001E+00
6 1.0000E+00 7 1.0001E+00
```

```
1 6.9039E-03 2 6.9039E-03 3 1.5745E-03 4 2.7586E-03 5 1.3310E-01
6 -1.3983E-01 7 -1.4164E-03 8 7.6472E-03 9 7.6472E-03 10 -6.7437E-05
11 3.2926E-03 12 2.1470E-03 13 2.5560E-04 14 2.9506E-03 15 6.0313E-04
16 1.2088E-03 17 1.2088E-03 18 1.3409E-04 19 1.4165E-03 20 1.3409E-04
21 1.4165E-03 22 -2.1840E-03 23 1.7680E-03 24 3.3372E-03 25 3.3146E-04
26 -2.6628E-03 27 3.2524E-03 28 -1.4140E-03 29 3.8295E-03 30 -1.3478E-02
31 -3.0855E-02 32 -6.3336E-04 33 4.3684E-02 34 6.7408E-02 35 3.5765E-02
36 -8.4872E-02 37 1.1726E-02 38 -5.6892E-02 39 2.1632E-03 40 2.0734E-02
41 1.5714E-02 42 9.1017E-03 43 2.8977E-03 44 -2.8983E-03 45 -1.0286E-02
46 -1.7266E-02 47 -2.5837E-02
```

THE SUM OF SQUARES IS 5.88738857E-02

PARROT: @@ No change in the parameters, check the diagram again

PARROT: mac tcex36cpd

... the command in full is MACRO\_FILE\_OPEN

PARROT: set-echo

NO SUCH COMMAND, USE HELP

PARROT: @@ Calculate the phase diagram

PARROT: @@ This TCM should be run in PARROT

PARROT: go p-3

... the command in full is GOTO\_MODULE

POLY\_3:

POLY\_3: @@ In PARROT, the global minimization is turned off automatically.

POLY\_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning

POLY\_3: @@ message will be given.

POLY\_3:

POLY\_3: advanced-option global yes,,

... the command in full is ADVANCED\_OPTIONS

Settings for global minimization:

\*\*\* WARNING \*\*\* Global equilibrium calculation may create new composition sets and this may corrupt your PARROT work file (.PAR file).

Do not go back to PARROT but exit from POLY after your POLY calculations.

POLY\_3:

POLY\_3: def-com,,,,

... the command in full is DEFINE\_COMPONENTS

POLY\_3: s-a-v 1 w(b) 0 1,,,,

... the command in full is SET\_AXIS\_VARIABLE

The condition W(B)=.1234 created

POLY\_3: s-a-v 2 t 300 1700,,,,

... the command in full is SET\_AXIS\_VARIABLE

The condition T=942.2 created

POLY\_3: s-c t=500

... the command in full is SET\_CONDITION

POLY\_3: l-c

... the command in full is LIST\_CONDITIONS

W(B)=0.1234, P=1E5, N=1, T=500

DEGREES OF FREEDOM 0

POLY\_3: c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Using global minimization procedure

Calculated 412 grid points in 0 s

Found the set of lowest grid points in 0 s

Calculated POLY solution 0 s, total time 0 s

POLY\_3: save tcex36 y

... the command in full is SAVE\_WORKSPACES

This file contains results from a previous STEP or MAP command.

The SAVE command will save the current status of the program but destroy the results from the previous STEP or MAP commands.

POLY\_3: map



Version S mapping is selected  
Generating start equilibrium 1  
Generating start equilibrium 2  
Generating start equilibrium 3  
Generating start equilibrium 4  
Generating start equilibrium 5  
Generating start equilibrium 6  
Generating start equilibrium 7  
Generating start equilibrium 8  
Generating start equilibrium 9  
Generating start equilibrium 10  
Generating start equilibrium 11  
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1  
Generating start point 2  
Generating start point 3  
Generating start point 4  
Generating start point 5  
Generating start point 6  
Generating start point 7  
Generating start point 8  
Generating start point 9  
Generating start point 10

Working hard

Generating start point 11  
Generating start point 12  
Generating start point 13  
Generating start point 14  
Generating start point 15  
Generating start point 16  
Generating start point 17  
Generating start point 18  
Generating start point 19  
Generating start point 20

Working hard

Generating start point 21  
Generating start point 22  
Generating start point 23  
Generating start point 24  
Generating start point 25  
Generating start point 26  
Generating start point 27  
Generating start point 28

Phase region boundary 1 at: 7.140E-01 3.100E+02  
BCC  
\*\* BCC#2  
Calculated.. 2 equilibria  
Terminating at axis limit.

Phase region boundary 2 at: 7.141E-01 3.000E+02  
BCC  
\*\* BCC#2  
Calculated. 14 equilibria

Phase region boundary 3 at: 6.817E-01 7.266E+02  
\*\* A2B  
BCC  
\*\* BCC#2

Phase region boundary 4 at: 3.625E-01 7.266E+02  
\*\* A2B  
BCC  
Calculated. 15 equilibria

Phase region boundary 5 at: 3.778E-01 1.185E+03  
\*\* LIQUID  
\*\* A2B  
BCC

Phase region boundary 6 at: 2.887E-01 1.185E+03  
\*\* LIQUID  
BCC  
Calculated 25 equilibria

Phase region boundary 7 at: 4.900E-01 1.185E+03  
\*\* LIQUID  
A2B  
Calculated. 33 equilibria

Phase region boundary 8 at: 6.482E-01 1.039E+03  
\*\* LIQUID  
A2B  
\*\* BCC

Phase region boundary 9 at: 7.637E-01 1.039E+03  
A2B  
\*\* BCC  
Calculated. 10 equilibria  
Terminating at known equilibrium

Phase region boundary 10 at: 8.259E-01 1.039E+03  
LIQUID  
\*\* BCC  
Calculated. 8 equilibria

Phase region boundary 11 at: 8.758E-01 1.204E+03  
LIQUID  
\*\* BCC  
\*\* FCC

Phase region boundary 12 at: 8.811E-01 1.204E+03  
LIQUID  
\*\* FCC  
Calculated 33 equilibria

Phase region boundary 13 at: 9.361E-01 1.204E+03  
BCC  
\*\* FCC  
Calculated 18 equilibria

Phase region boundary 14 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 15 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 16 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 17 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 18 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 19 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 20 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 21 at: 7.140E-01 3.100E+02  
 \*\* BCC  
 BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 22 at: 7.140E-01 3.100E+02  
 \*\* BCC  
 BCC#2  
 Calculated. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 23 at: 7.140E-01 3.100E+02  
 \*\* BCC  
 BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 24 at: 7.140E-01 3.100E+02  
 \*\* BCC  
 BCC#2  
 Calculated. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 25 at: 3.646E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated 10 equilibria

Phase region boundary 26 at: 3.646E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated. 3 equilibria  
 Terminating at known equilibrium

Phase region boundary 27 at: 3.646E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 28 at: 7.909E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated 10 equilibria

Phase region boundary 29 at: 7.909E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated. 3 equilibria  
 Terminating at known equilibrium

Phase region boundary 30 at: 7.909E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated. 9 equilibria  
 Terminating at known equilibrium

Phase region boundary 31 at: 2.435E-01 1.230E+03  
 \*\* LIQUID  
 BCC  
 Calculated. 4 equilibria  
 Terminating at known equilibrium

Phase region boundary 32 at: 2.435E-01 1.230E+03  
 \*\* LIQUID  
 BCC  
 Calculated 26 equilibria

```

Phase region boundary 33 at: 8.867E-01 1.230E+03
** LIQUID
FCC
Calculated. 2 equilibria
Terminating at known equilibrium

Phase region boundary 34 at: 8.867E-01 1.230E+03
** LIQUID
FCC
Calculated 29 equilibria

Phase region boundary 35 at: 6.404E-03 1.397E+03
LIQUID
** BCC
Calculated 11 equilibria

Phase region boundary 36 at: 6.404E-03 1.397E+03
LIQUID
** BCC
Calculated. 13 equilibria
Terminating at known equilibrium

Phase region boundary 37 at: 2.295E-01 1.243E+03
LIQUID
** BCC
Calculated 22 equilibria

Phase region boundary 38 at: 2.295E-01 1.243E+03
LIQUID
** BCC
Calculated. 4 equilibria
Terminating at known equilibrium

Phase region boundary 39 at: 6.122E-01 1.215E+03
LIQUID
** A2B
Calculated. 12 equilibria
Terminating at known equilibrium

Phase region boundary 40 at: 6.122E-01 1.215E+03
LIQUID
** A2B
Calculated. 8 equilibria
Terminating at known equilibrium

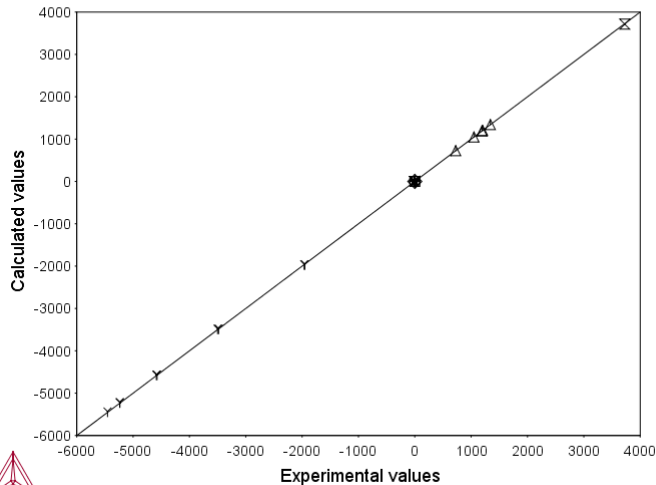
Phase region boundary 41 at: 9.927E-01 1.613E+03
LIQUID
** FCC
Calculated. 19 equilibria
Terminating at known equilibrium

Phase region boundary 42 at: 9.927E-01 1.613E+03
LIQUID
** FCC
Calculated 14 equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tce
x36.POLY3
CPU time for mapping 1 seconds
POLY_3: post
POST: s-l d
... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
... the command in full is PLOT DIAGRAM

```

#### From PARROT optimization

2016.05.16.14.21.39  
A,B  
P=1E5,N=1



- △ 1: T
- 2: W(LIQUID)
- ◇ 3: W(BCC,B)
- ⊗ 4: HTR
- ▽ 5: W(LIQUID)
- + 6: W(BCC,A)
- \* 7: W(FCC,A)
- × 8: X(BCC,B)
- 9: X(BCC#2)
- ★ 10: ACR(B)
- Υ 11: HMR(LIC)
- ⊠ 12:
- ⊗ 13:
- \* 14:
- ◆ 15:
- ⊕ 16: DGM
- △ 17: inequal
- 20: others

```

POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST: Hit RETURN to continue
POST: ba
... the command in full is BACK
POLY_3: ba
... the command in full is BACK

PARROT VERSION 5.3

Global minimization used as test only
PARROT: @@ Turn off alternate mode and try to calculate all equilibria
PARROT: s-alt Y
... the command in full is SET_ALTERNATE_MODE
Alternate calculation is on
PARROT: ed
... the command in full is EDIT_EXPERIMENTS

```

```

ED_EXP: read 1
... the command in full is READ_WORKSPACES
ED_EXP: c-a
... the command in full is COMPUTE_ALL_EQUILIBRIA
Eq Lab Iter Weight Temp Exp Fix phases or comments
1 AINV 4 1. 1184.6 LIQUID A2B BCC
2 AINV 2 1. 1314.5 LIQUID A2B
3 AINV 3 1. 1039.0 LIQUID A2B BCC
4 AINV 3 1. 1204.2 LIQUID BCC FCC
5 AINV 3 1. 726.6 A2B BCC BCC#2
6 AINV 3 1. 726.0 BCC BCC#2
10 ALF < unused > 1594.0 LIQUID FCC
11 ALF < unused > 1548.0 LIQUID FCC
12 ALF < unused > 1499.0 LIQUID FCC
13 ALF < unused > 1438.0 LIQUID FCC
20 ATIE 3 1. 1413.0 LIQUID FCC
21 ATIE 3 1. 1337.0 LIQUID FCC
22 ATIE 3 1. 1213.0 LIQUID FCC
23 ATIE 3 1. 1100.0 LIQUID BCC
100 AA 2 1. 1573.0 LIQUID
101 AA 2 1. 1573.0 LIQUID
102 AA 2 1. 1573.0 LIQUID
103 AA 2 1. 1573.0 LIQUID
104 AA 2 1. 1573.0 LIQUID
105 AA 2 1. 1573.0 LIQUID
106 AA 2 1. 1573.0 LIQUID
107 AA 2 1. 1573.0 LIQUID
108 AA 2 1. 1573.0 LIQUID
110 AH 2 1. 1773.0 LIQUID
111 AH 2 1. 1773.0 LIQUID
112 AH 2 1. 1773.0 LIQUID
113 AH 2 1. 1773.0 LIQUID
114 AH 2 1. 1773.0 LIQUID
115 AH 2 1. 1773.0 LIQUID
116 AH 2 1. 1773.0 LIQUID
117 AH 2 1. 1773.0 LIQUID
118 AH 2 1. 1773.0 LIQUID
ED_EXP: @@ Remove the equilibria with just liquid as we do not optimize
ED_EXP: @@ any liquid parameters and restore those with label ALF
ED_EXP: s-we 0 100-118
... the command in full is SET_WEIGHT
ED_EXP: s-we 1 alf
... the command in full is SET_WEIGHT
Changed weight on 4 equilibria.
ED_EXP: s-e 1
... the command in full is SELECT_EQUILIBRIUM
Equilibrium number 1, label AINV
ED_EXP: c-a
... the command in full is COMPUTE_ALL_EQUILIBRIA
Eq Lab Iter Weight Temp Exp Fix phases or comments
1 AINV 2 1. 1184.6 LIQUID A2B BCC
2 AINV 2 1. 1314.5 LIQUID A2B
3 AINV 2 1. 1039.0 LIQUID A2B BCC
4 AINV 2 1. 1204.2 LIQUID BCC FCC
5 AINV 2 1. 726.6 A2B BCC BCC#2
6 AINV 2 1. 726.0 BCC BCC#2
10 ALF 3 1. 1594.0 LIQUID FCC
11 ALF 3 1. 1548.0 LIQUID FCC
12 ALF 3 1. 1499.0 LIQUID FCC
13 ALF 3 1. 1438.0 LIQUID FCC
20 ATIE 2 1. 1413.0 LIQUID FCC
21 ATIE 2 1. 1337.0 LIQUID FCC
22 ATIE 2 1. 1213.0 LIQUID FCC
23 ATIE 2 1. 1100.0 LIQUID BCC
100 AA < unused > 1573.0 LIQUID
101 AA < unused > 1573.0 LIQUID
102 AA < unused > 1573.0 LIQUID
103 AA < unused > 1573.0 LIQUID
104 AA < unused > 1573.0 LIQUID
105 AA < unused > 1573.0 LIQUID
106 AA < unused > 1573.0 LIQUID
107 AA < unused > 1573.0 LIQUID
108 AA < unused > 1573.0 LIQUID
110 AH < unused > 1773.0 LIQUID
111 AH < unused > 1773.0 LIQUID
112 AH < unused > 1773.0 LIQUID
113 AH < unused > 1773.0 LIQUID
114 AH < unused > 1773.0 LIQUID
115 AH < unused > 1773.0 LIQUID
116 AH < unused > 1773.0 LIQUID
117 AH < unused > 1773.0 LIQUID
118 AH < unused > 1773.0 LIQUID
ED_EXP: save
... the command in full is SAVE_WORKSPACES
ED_EXP: @@ Save changes
ED_EXP: ba
... the command in full is BACK
PARROT: opt 0
... the command in full is OPTIMIZE_VARIABLES
Use 29 experiments, maximum is 2000
Use 554 real workspace, maximum is 50000
PARROT: l-r C SCREEN
... the command in full is LIST_RESULT

```

```

=====
OUTPUT FROM P A R R O T. DATE 2016. 5.16 14:21:40

```

```

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 0

```

```

== OPTIMIZING CONDITIONS ==

```

```

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 0 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

```

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.02809885E+04	2.02809885E+04	2.02809885E+04	7.39143651E-02
V2	-2.92651699E+01	-2.92651699E+01	-2.92651699E+01	3.41787474E-01
V11	-2.18102047E+04			
V12	1.51613087E+01			
V15	2.43700033E+04	2.43700033E+04	2.43700033E+04	6.09487672E-01
V16	-8.56548802E+00	-8.56463156E+00	-8.56463156E+00	2.04922287E+00
V17	3.11527172E+03	3.11496022E+03	3.11496022E+03	1.45833479E+00
V19	2.19570764E+04	2.19570764E+04	2.19570764E+04	4.63522316E+00
V20	-7.01233415E+00	-7.01163299E+00	-7.01163299E+00	1.12486774E+01

NUMBER OF OPTIMIZING VARIABLES : 7

ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO

THE SUM OF SQUARES HAS CHANGED FROM 5.88744378E-02 TO 8.99443380E+00

DEGREES OF FREEDOM 22. REDUCED SUM OF SQUARES 4.08837900E-01

SYMBOL	STATUS	VALUE/FUNCTION
1 R	80000000	8.3145100E+00
2 RTLNP	20000000	+R*T*LN(1E-05*P)
3 V1	48000000	2.0280989E+04
4 V2	48000000	-2.9265170E+01
13 V11	48000000	-2.1810205E+04
14 V12	48000000	1.5161309E+01
17 V15	48000000	2.4370003E+04
18 V16	48000000	-8.5654880E+00
19 V17	48000000	3.1152717E+03
21 V19	48000000	2.1957076E+04
22 V20	48000000	-7.0123342E+00

LIQUID

EXCESS MODEL IS REDLICH-KISTER\_MUGGIANU

CONSTITUENTS: A,B

G(LIQUID,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +14000-10\*T  
G(LIQUID,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +18000-12\*T  
L(LIQUID,A,B;0) = 500.00<T< 2000.00: +V11+V12\*T  
L(LIQUID,A,B;1) = 500.00<T< 2000.00: +V13+V14\*T

A2B

2 SUBLATTICES, SITES 2: 1

CONSTITUENTS: A : B

G(A2B,A;B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =  
500.00<T< 2000.00: +V1+V2\*T+V3\*T\*LN(T)

BCC

EXCESS MODEL IS REDLICH-KISTER\_MUGGIANU

CONSTITUENTS: A,B

G(BCC,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +0.0  
G(BCC,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +0.0  
L(BCC,A,B;0) = 500.00<T< 2000.00: +V15+V16\*T  
L(BCC,A,B;1) = 500.00<T< 2000.00: +V17+V18\*T

FCC

EXCESS MODEL IS REDLICH-KISTER\_MUGGIANU

CONSTITUENTS: A,B

G(FCC,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +408  
G(FCC,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +3300-3\*T  
L(FCC,A,B;0) = 500.00<T< 2000.00: +V19+V20\*T  
L(FCC,A,B;1) = 500.00<T< 2000.00: +V21+V22\*T

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS

DX=2E-2, P0=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%

HTR=HM(LIQUID)-HM(A2B)

1 T=1193	1185.	10.0	-8.445	-0.8445
1 W(LIQUID,B)=0.408	0.4163	2.00E-02	8.3025E-03	0.4151
1 W(BCC,B)=0.13	0.1322	2.00E-02	2.2006E-03	0.1100
2 T=1341	1315.	10.0	-26.49	-2.649
2 HTR=3727	3726.	5.00E+02	-0.7083	-1.4167E-03
3 T=1049	1039.	10.0	-10.03	-1.003
3 W(LIQUID,A)=0.27	0.2735	2.00E-02	3.4728E-03	0.1736
3 W(BCC,A)=9.3E-2	9.3787E-02	2.00E-02	7.8737E-04	3.9368E-02
4 T=1203	1204.	10.0	1.179	0.1179
4 W(LIQUID,A)=0.19	0.1890	2.00E-02	-9.8135E-04	-4.9067E-02
4 W(BCC,A)=6.9E-2	6.8455E-02	2.00E-02	-5.4510E-04	-2.7255E-02
4 W(FCC,A)=6E-2	5.9376E-02	2.00E-02	-6.2387E-04	-3.1194E-02
5 T=726	726.6	10.0	0.6276	6.2757E-02
5 X(BCC,B)=3.7E-2	3.7255E-02	2.00E-02	2.5471E-04	1.2736E-02
5 X(BCC#2,A)=0.114	0.1144	2.00E-02	4.0100E-04	2.0050E-02
6 X(BCC,B)=3.7E-2	3.7078E-02	2.00E-02	7.8113E-05	3.9056E-03
6 X(BCC#2,A)=0.114	0.1140	2.00E-02	-3.4068E-05	-1.7034E-03
10 W(LIQUID,A)=2E-2	1.9384E-02	2.00E-02	-6.1575E-04	-3.0788E-02
11 W(LIQUID,A)=4.2E-2	4.1484E-02	2.00E-02	-5.1605E-04	-2.5802E-02
12 W(LIQUID,A)=6.5E-2	6.4387E-02	2.00E-02	-6.1266E-04	-3.0633E-02
13 W(LIQUID,A)=9.3E-2	9.2002E-02	2.00E-02	-9.9776E-04	-4.9888E-02
20 W(LIQUID,A)=0.104	0.1030	2.00E-02	-9.6497E-04	-4.8249E-02
20 W(FCC,A)=3.8E-2	3.7713E-02	2.00E-02	-2.8716E-04	-1.4358E-02
21 W(LIQUID,A)=0.136	0.1356	2.00E-02	-4.2474E-04	-2.1237E-02
21 W(FCC,A)=4.7E-2	4.6609E-02	2.00E-02	-3.9077E-04	-1.9538E-02
22 W(LIQUID,A)=0.187	0.1856	2.00E-02	-1.4041E-03	-7.0205E-02
22 W(FCC,A)=5.9E-2	5.8614E-02	2.00E-02	-3.8608E-04	-1.9304E-02
23 W(LIQUID,A)=0.245	0.2434	2.00E-02	-1.5869E-03	-7.9344E-02
23 W(BCC,A)=8.5E-2	8.4361E-02	2.00E-02	-6.3920E-04	-3.1960E-02

PARROT:

```

PARROT:Hit RETURN to continue
PARROT: @@ When we optimize zero times we sometimes find an error for equilibrium 4
PARROT: @@ It can be on the wrong side, at high A instead of high B. Try to correct
PARROT: @@ that in the edit module.
PARROT: ed
... the command in full is EDIT_EXPERIMENTS
ED_EXP: read 1
... the command in full is READ_WORKSPACES
ED_EXP: s-e 4
... the command in full is SELECT_EQUILIBRIUM
Equilibrium number      4 , label AINV
ED_EXP: s-a-s
... the command in full is SET_ALL_START_VALUES
T /1204.179217/: 1200
Automatic start values for phase constituents? /N/: N

Phase LIQUID
Major constituent(s) /b/: b

Phase BCC
Major constituent(s) /b/: b

Phase FCC
Major constituent(s) /b/: b
ED_EXP:
ED_EXP: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Testing result with global minimization
13 ITS, CPU TIME USED 0 SECONDS
ED_EXP: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
Output from POLY-3, equilibrium =      4, label AINV, database:

Conditions:
P=1.01325E5
FIXED PHASES
LIQUID=1 BCC=1      FCC=1
DEGREES OF FREEDOM 0

Temperature 1204.18 K ( 931.03 C), Pressure 1.013250E+05
Number of moles of components 3.00000E+00, Mass in grams 1.30210E+02
Total Gibbs energy -9.82098E+03, Enthalpy 1.98581E+04, Volume 0.00000E+00

Component      Moles      W-Fraction Activity Potential Ref.stat
A      6.5966E-01  1.0132E-01 3.8855E-01 -9.4648E+03 SER
B      2.3403E+00  8.9868E-01 8.5841E-01 -1.5286E+03 SER

FCC      Status FIXED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 4.5911E+01, Volume fraction 0.0000E+00 Mass fractions:
B 9.40624E-01 A 5.93761E-02

BCC      Status FIXED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 4.5344E+01, Volume fraction 0.0000E+00 Mass fractions:
B 9.31545E-01 A 6.84549E-02

LIQUID      Status FIXED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 3.8955E+01, Volume fraction 0.0000E+00 Mass fractions:
B 8.10981E-01 A 1.89019E-01

EXPERIMENT T=1203:DT $1204.18:10 NO=1
EXPERIMENT W(LIQUID,A)=0.19:DX $0.189019:2E-2 NO=2
EXPERIMENT W(BCC,A)=6.9E-2:DX $6.84549E-2:2E-2 NO=3
EXPERIMENT W(FCC,A)=6E-2:DX $5.93761E-2:2E-2 NO=4
ED_EXP: ba
... the command in full is BACK
PARROT: @@ The error is still there, calculate the phase diagram!!!
PARROT: mac tcex36cpd
... the command in full is MACRO_FILE_OPEN
PARROT: set-echo
NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
... the command in full is GOTO_MODULE
POLY_3:
POLY_3: @@ In PARROT, the global minimization is turned off automatically.
POLY_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY_3: @@ message will be given.
POLY_3:
POLY_3: advanced-option global yes,,
... the command in full is ADVANCED_OPTIONS
Settings for global minimization:
*** WARNING *** Global equilibrium calculation may create new composition sets
and this may corrupt your PARROT work file (.PAR file).
Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY_3:
POLY_3: def-com,,,,
... the command in full is DEFINE_COMPONENTS
POLY_3: s-a-v 1 w(b) 0 1,,,,
... the command in full is SET_AXIS_VARIABLE
The condition W(B)=.1234 created
POLY_3: s-a-v 2 t 300 1700,,,,
... the command in full is SET_AXIS_VARIABLE
The condition T=942.2 created
POLY_3: s-c t=500
... the command in full is SET_CONDITION
POLY_3: l-c
... the command in full is LIST_CONDITIONS
W(B)=0.1234, P=1E5, N=1, T=500
DEGREES OF FREEDOM 0
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      412 grid points in      0 s
Found the set of lowest grid points in      0 s
Calculated POLY solution      0 s, total time      0 s
POLY_3: save tcex36 y
... the command in full is SAVE_WORKSPACES

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

```

```

POLY 3: map
Version 8 mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

Phase region boundary 1 at: 7.140E-01 3.100E+02
BCC
** BCC#2
Calculated.. 2 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 7.141E-01 3.000E+02
BCC
** BCC#2
Calculated. 14 equilibria

Phase region boundary 3 at: 6.817E-01 7.266E+02
** A2B
BCC
** BCC#2

Phase region boundary 4 at: 3.625E-01 7.266E+02
** A2B
BCC
Calculated. 15 equilibria

Phase region boundary 5 at: 3.778E-01 1.185E+03
** LIQUID
** A2B
BCC

Phase region boundary 6 at: 2.887E-01 1.185E+03
** LIQUID
BCC
Calculated 25 equilibria

Phase region boundary 7 at: 4.900E-01 1.185E+03
** LIQUID
A2B
Calculated. 33 equilibria

Phase region boundary 8 at: 6.482E-01 1.039E+03
** LIQUID
A2B
** BCC

Phase region boundary 9 at: 7.637E-01 1.039E+03
A2B
** BCC
Calculated. 10 equilibria
Terminating at known equilibrium

Phase region boundary 10 at: 8.259E-01 1.039E+03
LIQUID
** BCC
Calculated. 8 equilibria

Phase region boundary 11 at: 8.758E-01 1.204E+03
LIQUID
** BCC
** FCC

Phase region boundary 12 at: 8.811E-01 1.204E+03
LIQUID
** FCC
Calculated 33 equilibria

Phase region boundary 13 at: 9.361E-01 1.204E+03
BCC
** FCC

```

Calculated 18 equilibria

Phase region boundary 14 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 15 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 16 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 17 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 18 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 19 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 20 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 21 at: 7.140E-01 3.100E+02  
 \*\* BCC  
 BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 22 at: 7.140E-01 3.100E+02  
 \*\* BCC  
 BCC#2  
 Calculated. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 23 at: 7.140E-01 3.100E+02  
 \*\* BCC  
 BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 24 at: 7.140E-01 3.100E+02  
 \*\* BCC  
 BCC#2  
 Calculated. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 25 at: 3.646E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated 10 equilibria

Phase region boundary 26 at: 3.646E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated. 3 equilibria  
 Terminating at known equilibrium

Phase region boundary 27 at: 3.646E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 28 at: 7.909E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated 10 equilibria

Phase region boundary 29 at: 7.909E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated. 3 equilibria  
 Terminating at known equilibrium

Phase region boundary 30 at: 7.909E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated. 9 equilibria  
 Terminating at known equilibrium

Phase region boundary 31 at: 2.435E-01 1.230E+03  
 \*\* LIQUID  
 BCC  
 Calculated. 4 equilibria  
 Terminating at known equilibrium

Phase region boundary 32 at: 2.435E-01 1.230E+03  
 \*\* LIQUID  
 BCC



```

Calculated                26 equilibria

Phase region boundary 33 at:  8.867E-01  1.230E+03
** LIQUID
   FCC
Calculated.                2 equilibria
Terminating at known equilibrium

Phase region boundary 34 at:  8.867E-01  1.230E+03
** LIQUID
   FCC
Calculated                29 equilibria

Phase region boundary 35 at:  6.404E-03  1.397E+03
   LIQUID
** BCC
Calculated                11 equilibria

Phase region boundary 36 at:  6.404E-03  1.397E+03
   LIQUID
** BCC
Calculated.                13 equilibria
Terminating at known equilibrium

Phase region boundary 37 at:  2.295E-01  1.243E+03
   LIQUID
** BCC
Calculated                22 equilibria

Phase region boundary 38 at:  2.295E-01  1.243E+03
   LIQUID
** BCC
Calculated.                4 equilibria
Terminating at known equilibrium

Phase region boundary 39 at:  6.122E-01  1.215E+03
   LIQUID
** A2B
Calculated.                12 equilibria
Terminating at known equilibrium

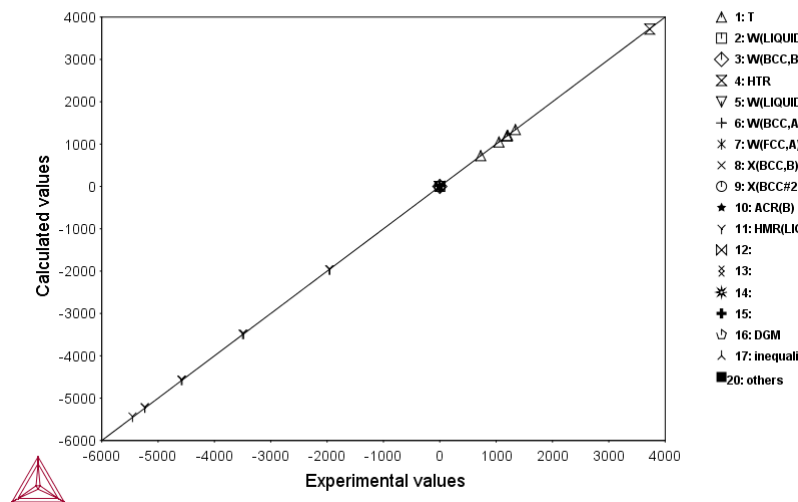
Phase region boundary 40 at:  6.122E-01  1.215E+03
   LIQUID
** A2B
Calculated.                8 equilibria
Terminating at known equilibrium

Phase region boundary 41 at:  9.927E-01  1.613E+03
   LIQUID
** FCC
Calculated.                19 equilibria
Terminating at known equilibrium

Phase region boundary 42 at:  9.927E-01  1.613E+03
   LIQUID
** FCC
Calculated                14 equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tce
x36.POLY3
CPU time for mapping                1 seconds
POLY_3: post
POST: s-l d
... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
... the command in full is PLOT DIAGRAM
From PARROT optimization

2016.05.16.14.21.44
A,B
P=1E5,N=1

```



```

POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:Hit RETURN to continue
POST: @@ The phase diagram shows there is no equilibrium between liquid,
POST: @@ fcc and bcc at high B content. For the moment we better remove
POST: @@ equilibrium 4 from the optimization.
POST: ba
... the command in full is BACK
POLY_3: ba
... the command in full is BACK

PARROT VERSION 5.3

Global minimization used as test only
PARROT: ed

```

```

... the command in full is EDIT_EXPERIMENTS
ED_EXP: read 1
... the command in full is READ_WORKSPACES
ED_EXP: s-we 0 4
... the command in full is SET_WEIGHT
ED_EXP: save
... the command in full is SAVE_WORKSPACES
ED_EXP: ba
... the command in full is BACK
PARROT: opt 0
... the command in full is OPTIMIZE_VARIABLES
Use      25 experiments, maximum is      2000
Use     494 real workspace, maximum is    50000
PARROT: l-r C SCREEN
... the command in full is LIST_RESULT

```

```

=====
OUTPUT FROM P A R R O T.  DATE 2016. 5.16   14:21:45

```

```

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 0

```

```

== OPTIMIZING CONDITIONS ==

```

```

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 0 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

```

```

== OPTIMIZING VARIABLES ==

```

```

AVAILABLE VARIABLES ARE V1 TO V00

```

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.02809885E+04	2.02809885E+04	2.02809885E+04	7.39143651E-02
V2	-2.92651699E+01	-2.92651699E+01	-2.92651699E+01	3.41787474E-01
V11	-2.18102047E+04			
V12	1.51613087E+01			
V15	2.43700033E+04	2.43700033E+04	2.43700033E+04	6.09487672E-01
V16	-8.56548802E+00	-8.56463156E+00	-8.56463156E+00	2.04922287E+00
V17	3.11527172E+03	3.11496022E+03	3.11496022E+03	1.45833479E+00
V19	2.19570764E+04	2.19570764E+04	2.19570764E+04	4.63522316E+00
V20	-7.01233415E+00	-7.01163299E+00	-7.01163299E+00	1.12486774E+01

```

NUMBER OF OPTIMIZING VARIABLES : 7
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 5.88744378E-02 TO 8.97640476E+00
DEGREES OF FREEDOM 18. REDUCED SUM OF SQUARES 4.98689154E-01

```

SYMBOL	STATUS	VALUE/FUNCTION
1 R	80000000	8.3145100E+00
2 RTLNP	20000000	+R*T*LN(1E-05*P)
3 V1	48000000	2.0280989E+04
4 V2	48000000	-2.9265170E+01
13 V11	48000000	-2.1810205E+04
14 V12	48000000	1.5161309E+01
17 V15	48000000	2.4370003E+04
18 V16	48000000	-8.5654880E+00
19 V17	48000000	3.1152717E+03
21 V19	48000000	2.1957076E+04
22 V20	48000000	-7.0123342E+00

```

LIQUID
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
CONSTITUENTS: A,B

```

```

G(LIQUID,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +14000-10*T
G(LIQUID,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +18000-12*T
L(LIQUID,A,B;0) = 500.00<T< 2000.00: +V11+V12*T
L(LIQUID,A,B;1) = 500.00<T< 2000.00: +V13+V14*T

```

```

A2B
2 SUBLATTICES, SITES 2: 1
CONSTITUENTS: A : B

```

```

G(A2B,A;B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =
500.00<T< 2000.00: +V1+V2*T+V3*T*LN(T)

```

```

BCC
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
CONSTITUENTS: A,B

```

```

G(BCC,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +0.0
G(BCC,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +0.0
L(BCC,A,B;0) = 500.00<T< 2000.00: +V15+V16*T
L(BCC,A,B;1) = 500.00<T< 2000.00: +V17+V18*T

```

```

FCC
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
CONSTITUENTS: A,B

```

```

G(FCC,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +408
G(FCC,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +3300-3*T
L(FCC,A,B;0) = 500.00<T< 2000.00: +V19+V20*T
L(FCC,A,B;1) = 500.00<T< 2000.00: +V21+V22*T

```

```

$ ===== BLOCK NUMBER 1

```

```

DEFINED CONSTANTS
  DX=2E-2, P0=101325, DH=500, DT=10
DEFINED FUNCTIONS AND VARIABLES%
  HTR=HM(LIQUID)-HM(A2B)
1 T=1193                1185.        10.0        -8.445        -0.8445
1 W(LIQUID,B)=0.408      0.4163      2.00E-02      8.3025E-03      0.4151
1 W(BCC,B)=0.13          0.1322      2.00E-02      2.2006E-03      0.1100
2 T=1341                1315.        10.0        -26.49        -2.649
2 HTR=3727              3726.        5.00E+02      -0.7083        -1.4167E-03
3 T=1049                1039.        10.0        -10.03        -1.003
3 W(LIQUID,A)=0.27       0.2735      2.00E-02      3.4728E-03      0.1736
3 W(BCC,A)=9.3E-2       9.3787E-02  2.00E-02      7.8737E-04      3.9368E-02
5 T=726                 726.6        10.0         0.6276        6.2757E-02
5 X(BCC,B)=3.7E-2       3.7255E-02  2.00E-02      2.5471E-04      1.2736E-02
5 X(BCC#2,A)=0.114      0.1144      2.00E-02      4.0100E-04      2.0050E-02
6 X(BCC,B)=3.7E-2       3.7078E-02  2.00E-02      7.8113E-05      3.9056E-03
6 X(BCC#2,A)=0.114      0.1140      2.00E-02      -3.4068E-05     -1.7034E-03
10 W(LIQUID,A)=2E-2      1.9384E-02  2.00E-02      -6.1575E-04     -3.0788E-02
11 W(LIQUID,A)=4.2E-2    4.1484E-02  2.00E-02      -5.1605E-04     -2.5802E-02
12 W(LIQUID,A)=6.5E-2    6.4387E-02  2.00E-02      -6.1266E-04     -3.0633E-02
13 W(LIQUID,A)=9.3E-2    9.2002E-02  2.00E-02      -9.9776E-04     -4.9888E-02
20 W(LIQUID,A)=0.104     0.1030      2.00E-02      -9.6497E-04     -4.8249E-02
20 W(FCC,A)=3.8E-2       3.7713E-02  2.00E-02      -2.8716E-04     -1.4358E-02
21 W(LIQUID,A)=0.136     0.1356      2.00E-02      -4.2474E-04     -2.1237E-02
21 W(FCC,A)=4.7E-2       4.6609E-02  2.00E-02      -3.9077E-04     -1.9538E-02
22 W(LIQUID,A)=0.187     0.1856      2.00E-02      -1.4041E-03     -7.0205E-02
22 W(FCC,A)=5.9E-2       5.8614E-02  2.00E-02      -3.8608E-04     -1.9304E-02
23 W(LIQUID,A)=0.245     0.2434      2.00E-02      -1.5869E-03     -7.9344E-02
23 W(BCC,A)=8.5E-2       8.4361E-02  2.00E-02      -6.3920E-04     -3.1960E-02

```

```

PARROT:
PARROT:Hit RETURN to continue
PARROT: opt 30
... the command in full is OPTIMIZE_VARIABLES
Use      25 experiments, maximum is      2000
Use     494 real workspace, maximum is    50000
The following output is provided by subroutine VA05A

```

```

      AT THE      0 TH ITERATION WE HAVE THE SUM OF SQUARES      8.97640476E+00
1  1.0000E+00    2  1.0000E+00    3  1.0000E+00    4  1.0001E+00    5  1.0001E+00
6  1.0000E+00    7  1.0001E+00

      AT THE      1 ST ITERATION WE HAVE THE SUM OF SQUARES      9.13900120E+00
1  1.0001E+00    2  1.0000E+00    3  1.0000E+00    4  1.0001E+00    5  1.0001E+00
6  1.0000E+00    7  1.0001E+00

      AT THE      2 ND ITERATION WE HAVE THE SUM OF SQUARES      8.68324796E+00
1  1.0000E+00    2  1.0001E+00    3  1.0000E+00    4  1.0001E+00    5  1.0001E+00
6  1.0000E+00    7  1.0001E+00

      AT THE      3 RD ITERATION WE HAVE THE SUM OF SQUARES      8.69026383E+00
1  1.0000E+00    2  1.0001E+00    3  1.0001E+00    4  1.0001E+00    5  1.0001E+00
6  1.0000E+00    7  1.0001E+00

      AT THE      4 TH ITERATION WE HAVE THE SUM OF SQUARES      8.68061561E+00
1  1.0000E+00    2  1.0001E+00    3  1.0000E+00    4  1.0002E+00    5  1.0001E+00
6  1.0000E+00    7  1.0001E+00

      AT THE      5 TH ITERATION WE HAVE THE SUM OF SQUARES      8.68025225E+00
1  1.0000E+00    2  1.0001E+00    3  1.0000E+00    4  1.0002E+00    5  1.0002E+00
6  1.0000E+00    7  1.0001E+00

      AT THE      6 TH ITERATION WE HAVE THE SUM OF SQUARES      8.68061354E+00
1  1.0000E+00    2  1.0001E+00    3  1.0000E+00    4  1.0002E+00    5  1.0002E+00
6  1.0001E+00    7  1.0001E+00

      AT THE      7 TH ITERATION WE HAVE THE SUM OF SQUARES      8.68010001E+00
1  1.0000E+00    2  1.0001E+00    3  1.0000E+00    4  1.0002E+00    5  1.0002E+00
6  1.0000E+00    7  1.0002E+00

      AT THE      8 TH ITERATION WE HAVE THE SUM OF SQUARES      4.74733287E-01
1  9.9763E-01    2  1.0044E+00    3  9.9990E-01    4  1.0002E+00    5  1.0002E+00
6  9.9999E-01    7  1.0002E+00

      AT THE      9 TH ITERATION WE HAVE THE SUM OF SQUARES      3.94612071E-01
1  9.9883E-01    2  1.0048E+00    3  9.9988E-01    4  1.0031E+00    5  1.0015E+00
6  1.0010E+00    7  1.0037E+00

      AT THE     10 TH ITERATION WE HAVE THE SUM OF SQUARES      3.39925250E-01
1  9.9933E-01    2  1.0054E+00    3  1.0002E+00    4  1.0049E+00    5  1.0023E+00
6  1.0045E+00    7  1.0127E+00

      AT THE     11 TH ITERATION WE HAVE THE SUM OF SQUARES      2.09925807E-01
1  1.0023E+00    2  1.0068E+00    3  1.0020E+00    4  1.0149E+00    5  1.0070E+00
6  9.9722E-01    7  9.9852E-01

      AT THE     12 TH ITERATION WE HAVE THE SUM OF SQUARES      1.27916004E-01
1  1.0072E+00    2  1.0096E+00    3  1.0064E+00    4  1.0333E+00    5  1.0153E+00
6  1.0040E+00    7  1.0210E+00

THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED      12 iterations
1  1.0072E+00    2  1.0096E+00    3  1.0064E+00    4  1.0333E+00    5  1.0153E+00
6  1.0040E+00    7  1.0210E+00

1 -1.2012E-01    2  1.6807E-02    3  7.7726E-02    4  7.5285E-02    5 -9.8949E-02
6 -1.6451E-01    7  5.6332E-02    8  1.1680E-01    9 -1.5429E-01   10 -1.7636E-02
11 3.4908E-02   12 4.0882E-03   13 8.9192E-02   14 -2.2047E-02   15 -9.2884E-03
16 -8.1454E-03   17 -2.2546E-02   18 -1.9582E-02   19 1.7801E-02   20 9.6277E-03
21 1.8367E-02   22 -3.9899E-02   23 2.5880E-02   24 9.1761E-03   25 9.9469E-02

```

```

      THE SUM OF SQUARES IS      1.27916004E-01
PARROT: cont 30
... the command in full is CONTINUE_OPTIMIZATION

It is safe to CONTINUE only after TOO MANY ITERATIONS
and no change in variables and experiments ...
Now anything can happen ...

PARROT: l-r C SCREEN
... the command in full is LIST_RESULT

```

```

=====

```

\*\*\* SUCCESSFUL OPTIMIZATION. \*\*\*  
NUMBER OF ITERATIONS: 13

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N  
MINIMUM SAVE ON FILE: Y  
ERROR FOR INEQUALITIES = 1.00000000E+00  
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04  
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)  
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04  
ACC = (INITIAL SUM OF SQUARES) \* 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.04272876E+04	2.02809885E+04	2.02809885E+04	2.59209705E-02
V2	-2.95468613E+01	-2.92651699E+01	-2.92651699E+01	1.40177728E-02
V11	-2.18102047E+04			
V12	1.51613087E+01			
V15	2.45250655E+04	2.43700033E+04	2.43700033E+04	9.62418602E-02
V16	-8.85015072E+00	-8.56463156E+00	-8.56463156E+00	2.78844062E-01
V17	3.16252983E+03	3.11496022E+03	3.11496022E+03	2.49147755E-01
V19	2.20441098E+04	2.19570764E+04	2.19570764E+04	6.73748360E-01
V20	-7.15892220E+00	-7.01163299E+00	-7.01163299E+00	1.60351723E+00

NUMBER OF OPTIMIZING VARIABLES : 7  
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO  
THE SUM OF SQUARES HAS CHANGED FROM 8.97640476E+00 TO 1.27916004E-01  
DEGREES OF FREEDOM 18. REDUCED SUM OF SQUARES 7.10644464E-03

SYMBOL	STATUS	VALUE/FUNCTION
1 R	80000000	8.3145100E+00
2 RTLNP	20000000	+R*T*LN(1E-05*P)
3 V1	48000000	2.0427288E+04
4 V2	48000000	-2.9546861E+01
13 V11	48000000	-2.1810205E+04
14 V12	48000000	1.5161309E+01
17 V15	48000000	2.4525066E+04
18 V16	48000000	-8.8501507E+00
19 V17	48000000	3.1625298E+03
21 V19	48000000	2.2044110E+04
22 V20	48000000	-7.1589222E+00

LIQUID  
EXCESS MODEL IS REDLICH-KISTER\_MUGGIANU  
CONSTITUENTS: A,B

G(LIQUID,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +14000-10\*T  
G(LIQUID,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +18000-12\*T  
L(LIQUID,A,B;0) = 500.00<T< 2000.00: +V11+V12\*T  
L(LIQUID,A,B;1) = 500.00<T< 2000.00: +V13+V14\*T

A2B  
2 SUBLATTICES, SITES 2: 1  
CONSTITUENTS: A : B

G(A2B,A;B;0) - 2 G(BCC,A;0) - G(BCC,B;0) =  
500.00<T< 2000.00: +V1+V2\*T+V3\*T\*LN(T)

BCC  
EXCESS MODEL IS REDLICH-KISTER\_MUGGIANU  
CONSTITUENTS: A,B

G(BCC,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +0.0  
G(BCC,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +0.0  
L(BCC,A,B;0) = 500.00<T< 2000.00: +V15+V16\*T  
L(BCC,A,B;1) = 500.00<T< 2000.00: +V17+V18\*T

FCC  
EXCESS MODEL IS REDLICH-KISTER\_MUGGIANU  
CONSTITUENTS: A,B

G(FCC,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +408  
G(FCC,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +3300-3\*T  
L(FCC,A,B;0) = 500.00<T< 2000.00: +V19+V20\*T  
L(FCC,A,B;1) = 500.00<T< 2000.00: +V21+V22\*T

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS

DX=2E-2, P0=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%

HTR=HM(LIQUID)-HM(A2B)

1 T=1193	1192.	10.0	-1.201	-0.1201
1 W(LIQUID,B)=0.408	0.4083	2.00E-02	3.3615E-04	1.6807E-02
1 W(BCC,B)=0.13	0.1316	2.00E-02	1.5545E-03	7.7726E-02
2 T=1341	1342.	10.0	0.7529	7.5285E-02
2 HTR=3727	3678.	5.00E+02	-49.47	-9.8949E-02
3 T=1049	1047.	10.0	-1.645	-0.1645
3 W(LIQUID,A)=0.27	0.2711	2.00E-02	1.1266E-03	5.6332E-02
3 W(BCC,A)=9.3E-2	9.5336E-02	2.00E-02	2.3361E-03	0.1168
5 T=726	724.5	10.0	-1.543	-0.1543
5 X(BCC,B)=3.7E-2	3.6647E-02	2.00E-02	-3.5272E-04	-1.7636E-02
5 X(BCC#2,A)=0.114	0.1147	2.00E-02	6.9816E-04	3.4908E-02
6 X(BCC,B)=3.7E-2	3.7082E-02	2.00E-02	8.1763E-05	4.0882E-03
6 X(BCC#2,A)=0.114	0.1158	2.00E-02	1.7838E-03	8.9192E-02

```

10 W(LIQUID,A)=2E-2          1.9559E-02  2.00E-02 -4.4094E-04 -2.2047E-02
11 W(LIQUID,A)=4.2E-2        4.1814E-02  2.00E-02 -1.8577E-04 -9.2884E-03
12 W(LIQUID,A)=6.5E-2        6.4837E-02  2.00E-02 -1.6291E-04 -8.1454E-03
13 W(LIQUID,A)=9.3E-2        9.2549E-02  2.00E-02 -4.5092E-04 -2.2546E-02
20 W(LIQUID,A)=0.104         0.1036      2.00E-02 -3.9164E-04 -1.9582E-02
20 W(FCC,A)=3.8E-2           3.8356E-02  2.00E-02  3.5602E-04  1.7801E-02
21 W(LIQUID,A)=0.136         0.1362      2.00E-02  1.9255E-04  9.6277E-03
21 W(FCC,A)=4.7E-2           4.7367E-02  2.00E-02  3.6734E-04  1.8367E-02
22 W(LIQUID,A)=0.187         0.1862      2.00E-02 -7.9799E-04 -3.9899E-02
22 W(FCC,A)=5.9E-2           5.9518E-02  2.00E-02  5.1760E-04  2.5880E-02
23 W(LIQUID,A)=0.245         0.2452      2.00E-02  1.8352E-04  9.1761E-03
23 W(BCC,A)=8.5E-2           8.6989E-02  2.00E-02  1.9894E-03  9.9469E-02

```

```

PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ Optimization converged, try to add equilibrium 4 again
PARROT: ed
... the command in full is EDIT_EXPERIMENTS
ED_EXP: read 1
... the command in full is READ_WORKSPACES
ED_EXP: s-e 4
... the command in full is SELECT_EQUILIBRIUM
Equilibrium number      4 , label AINV
ED_EXP: s-a-s
... the command in full is SET_ALL_START_VALUES
T /1204.179217/: 1200
Automatic start values for phase constituents? /N/: N

Phase LIQUID
Major constituent(s) /b/: b

Phase BCC
Major constituent(s) /b/: b

Phase FCC
Major constituent(s) /b/: b
ED_EXP:
ED_EXP: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Testing result with global minimization
13 ITS, CPU TIME USED 0 SECONDS
ED_EXP: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
Output from POLY-3, equilibrium =      4, label AINV, database:

Conditions:
P=1.01325E5
FIXED PHASES
LIQUID=1 BCC=1 FCC=1
DEGREES OF FREEDOM 0

Temperature 1211.83 K ( 938.68 C), Pressure 1.013250E+05
Number of moles of components 3.00000E+00, Mass in grams 1.30242E+02
Total Gibbs energy -1.00413E+04, Enthalpy 1.99592E+04, Volume 0.00000E+00

Component      Moles      W-Fraction Activity Potential Ref.stat
A              6.5860E-01  1.0113E-01 3.8288E-01 -9.6731E+03 SER
B              2.3414E+00  8.9887E-01 8.5591E-01 -1.5677E+03 SER

FCC              Status FIXED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 4.5896E+01, Volume fraction 0.0000E+00 Mass fractions:
B 9.40380E-01 A 5.96204E-02

BCC              Status FIXED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 4.5283E+01, Volume fraction 0.0000E+00 Mass fractions:
B 9.30563E-01 A 6.94370E-02

LIQUID           Status FIXED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 3.9063E+01, Volume fraction 0.0000E+00 Mass fractions:
B 8.13344E-01 A 1.86656E-01

SET_WEIGHT 0,,,
EXPERIMENT T=1203:DT
EXPERIMENT W(LIQUID,A)=0.19:DX
EXPERIMENT W(BCC,A)=6.9E-2:DX
EXPERIMENT W(FCC,A)=6E-2:DX
ED_EXP: ba
... the command in full is BACK
PARROT: @@ It still fails, try to calculate the phase diagram again.
PARROT: mac tcex36cpd
... the command in full is MACRO_FILE_OPEN
PARROT: set-echo
NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
... the command in full is GOTO_MODULE
POLY_3:
POLY_3: @@ In PARROT, the global minimization is turned off automatically.
POLY_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY_3: @@ message will be given.
POLY_3:
POLY_3: advanced-option global yes,,
... the command in full is ADVANCED_OPTIONS
Settings for global minimization:
*** WARNING *** Global equilibrium calculation may create new composition sets
and this may corrupt your PARROT work file (.PAR file).
Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY_3:
POLY_3: def-com,,,,
... the command in full is DEFINE_COMPONENTS
POLY_3: s-a-v 1 w(b) 0 1,,,
... the command in full is SET_AXIS_VARIABLE
The condition W(B)=.1234 created
POLY_3: s-a-v 2 t 300 1700,,,
... the command in full is SET_AXIS_VARIABLE
The condition T=942.2 created
POLY_3: s-c t=500
... the command in full is SET_CONDITION
POLY_3: l-c
... the command in full is LIST_CONDITIONS

```

W(B)=0.1234, P=1E5, N=1, T=500  
DEGREES OF FREEDOM 0

**POLY\_3:** c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Using global minimization procedure

Calculated 412 grid points in 0 s

Found the set of lowest grid points in 0 s

Calculated POLY solution 0 s, total time 0 s

**POLY\_3:** save tcex36 y

... the command in full is SAVE\_WORKSPACES

This file contains results from a previous STEP or MAP command.

The SAVE command will save the current status of the program but destroy  
the results from the previous STEP or MAP commands.

**POLY\_3:** map

Version S mapping is selected

Generating start equilibrium 1

Generating start equilibrium 2

Generating start equilibrium 3

Generating start equilibrium 4

Generating start equilibrium 5

Generating start equilibrium 6

Generating start equilibrium 7

Generating start equilibrium 8

Generating start equilibrium 9

Generating start equilibrium 10

Generating start equilibrium 11

Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1

Generating start point 2

Generating start point 3

Generating start point 4

Generating start point 5

Generating start point 6

Generating start point 7

Generating start point 8

Generating start point 9

Generating start point 10

Working hard

Generating start point 11

Generating start point 12

Generating start point 13

Generating start point 14

Generating start point 15

Generating start point 16

Generating start point 17

Generating start point 18

Generating start point 19

Generating start point 20

Working hard

Generating start point 21

Generating start point 22

Generating start point 23

Generating start point 24

Generating start point 25

Generating start point 26

Generating start point 27

Generating start point 28

Phase region boundary 1 at: 7.140E-01 3.100E+02

BCC

\*\* BCC#2

Calculated.. 2 equilibria

Terminating at axis limit.

Phase region boundary 2 at: 7.141E-01 3.000E+02

BCC

\*\* BCC#2

Calculated. 14 equilibria

Phase region boundary 3 at: 6.813E-01 7.245E+02

\*\* A2B

BCC

\*\* BCC#2

Phase region boundary 4 at: 3.620E-01 7.245E+02

\*\* A2B

BCC

Calculated. 15 equilibria

Phase region boundary 5 at: 3.775E-01 1.192E+03

\*\* LIQUID

\*\* A2B

BCC

Phase region boundary 6 at: 2.837E-01 1.192E+03

\*\* LIQUID

BCC

Calculated 24 equilibria

Phase region boundary 7 at: 4.865E-01 1.192E+03

\*\* LIQUID

A2B

Calculated. 33 equilibria

Phase region boundary 8 at: 6.495E-01 1.047E+03

\*\* LIQUID

A2B

\*\* BCC

Phase region boundary 9 at: 7.626E-01 1.047E+03

A2B

\*\* BCC

Calculated. 11 equilibria

Terminating at known equilibrium

Phase region boundary 10 at: 8.259E-01 1.047E+03

LIQUID

\*\* BCC

Calculated. 9 equilibria

Phase region boundary 11 at: 8.763E-01 1.212E+03  
 LIQUID  
 \*\* BCC  
 \*\* FCC

Phase region boundary 12 at: 8.820E-01 1.212E+03  
 LIQUID  
 \*\* FCC  
 Calculated 35 equilibria

Phase region boundary 13 at: 9.355E-01 1.212E+03  
 BCC  
 \*\* FCC  
 Calculated 24 equilibria

Phase region boundary 14 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 15 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 16 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 17 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 18 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 19 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 20 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 21 at: 7.140E-01 3.100E+02  
 \*\* BCC  
 BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 22 at: 7.140E-01 3.100E+02  
 \*\* BCC  
 BCC#2  
 Calculated. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 23 at: 7.140E-01 3.100E+02  
 \*\* BCC  
 BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 24 at: 7.140E-01 3.100E+02  
 \*\* BCC  
 BCC#2  
 Calculated. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 25 at: 3.642E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated 10 equilibria

Phase region boundary 26 at: 3.642E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated. 3 equilibria  
 Terminating at known equilibrium

Phase region boundary 27 at: 3.642E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated. 14 equilibria  
 Terminating at known equilibrium

Phase region boundary 28 at: 7.905E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated 10 equilibria

Phase region boundary 29 at: 7.905E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated. 3 equilibria  
 Terminating at known equilibrium

Phase region boundary 30 at: 7.905E-01 7.700E+02

```

** A2B
  BCC
Calculated.          9 equilibria
Terminating at known equilibrium

Phase region boundary 31 at:  2.451E-01  1.230E+03
** LIQUID
  BCC
Calculated.          4 equilibria
Terminating at known equilibrium

Phase region boundary 32 at:  2.451E-01  1.230E+03
** LIQUID
  BCC
Calculated          26 equilibria

Phase region boundary 33 at:  8.859E-01  1.230E+03
** LIQUID
  FCC
Calculated.          2 equilibria
Terminating at known equilibrium

Phase region boundary 34 at:  8.859E-01  1.230E+03
** LIQUID
  FCC
Calculated          29 equilibria

Phase region boundary 35 at:  6.428E-03  1.397E+03
  LIQUID
** BCC
Calculated          8 equilibria

Phase region boundary 36 at:  6.428E-03  1.397E+03
  LIQUID
** BCC
Calculated.         13 equilibria
Terminating at known equilibrium

Phase region boundary 37 at:  2.303E-01  1.244E+03
  LIQUID
** BCC
Calculated          22 equilibria

Phase region boundary 38 at:  2.303E-01  1.244E+03
  LIQUID
** BCC
Calculated.          4 equilibria
Terminating at known equilibrium

Phase region boundary 39 at:  6.122E-01  1.239E+03
  LIQUID
** A2B
Calculated.         14 equilibria
Terminating at known equilibrium

Phase region boundary 40 at:  6.122E-01  1.239E+03
  LIQUID
** A2B
Calculated.          8 equilibria
Terminating at known equilibrium

Phase region boundary 41 at:  9.927E-01  1.613E+03
  LIQUID
** FCC
Calculated.         19 equilibria
Terminating at known equilibrium

Phase region boundary 42 at:  9.927E-01  1.613E+03
  LIQUID
** FCC
Calculated          9 equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tce
x36.POLY3
CPU time for mapping          1 seconds
POLY_3: post
POST: s-l d
... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
... the command in full is PLOT DIAGRAM

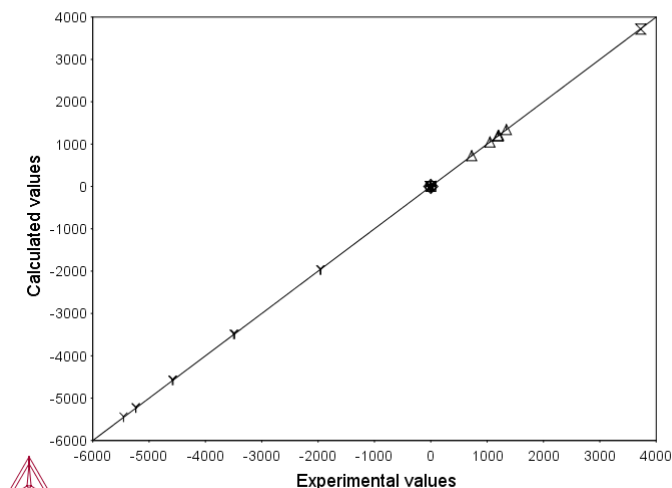
```

### From PARROT optimization

2016.05.16.14.21.49

A,B

P=1E5,N=1



- △ 1: T
- 2: W(LIQUID)
- ◇ 3: W(BCC,B)
- ⊗ 4: HTR
- ▽ 5: W(LIQUID)
- + 6: W(BCC,A)
- \* 7: W(FCC,A)
- × 8: X(BCC,B)
- 9: X(BCC#2)
- ★ 10: ACR(B)
- γ 11: HMR(LIQUID)
- ⊗ 12:
- ⊗ 13:
- \* 14:
- ⊕ 15:
- ⊕ 16: DGM
- ⊕ 17: inequality
- 20: others



POST: set-inter



```

... the command in full is SET_INTERACTIVE_MODE
POST:Hit RETURN to continue
POST: @@ Sometimes a very strange shape of the fcc phase here and no
POST: @@ equilibrium between liq, fcc and bcc at high B content.
POST: ba
... the command in full is BACK
POLY_3: ba
... the command in full is BACK

PARROT VERSION 5.3

Global minimization used as test only
PARROT: l-r C SCREEN
... the command in full is LIST_RESULT

=====
OUTPUT FROM P A R R O T. DATE 2016. 5.16 14:21:50

*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 13

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR. VALUE START VALUE SCALING FACTOR REL.STAND.DEV
V1 2.04272876E+04 2.02809885E+04 2.02809885E+04 2.59209705E-02
V2 -2.95468613E+01 -2.92651699E+01 -2.92651699E+01 1.40177728E-02
V11 -2.18102047E+04
V12 1.51613087E+01
V15 2.45250655E+04 2.43700033E+04 2.43700033E+04 9.62418602E-02
V16 -8.85015072E+00 -8.56463156E+00 -8.56463156E+00 2.78844062E-01
V17 3.16252983E+03 3.11496022E+03 3.11496022E+03 2.49147755E-01
V19 2.20441098E+04 2.19570764E+04 2.19570764E+04 6.73748360E-01
V20 -7.15892220E+00 -7.01163299E+00 -7.01163299E+00 1.60351723E+00

NUMBER OF OPTIMIZING VARIABLES : 7
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 8.97640476E+00 TO 1.27916004E-01
DEGREES OF FREEDOM 18. REDUCED SUM OF SQUARES 7.10644464E-03

SYMBOL STATUS VALUE/FUNCTION
1 R 80000000 8.3145100E+00
2 RTLNP 20000000 +R*T*LN(1E-05*P)
3 V1 48000000 2.0427288E+04
4 V2 48000000 -2.9546861E+01
13 V11 48000000 -2.1810205E+04
14 V12 48000000 1.5161309E+01
17 V15 48000000 2.4525066E+04
18 V16 48000000 -8.8501507E+00
19 V17 48000000 3.1625298E+03
21 V19 48000000 2.2044110E+04
22 V20 48000000 -7.1589222E+00

LIQUID
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
CONSTITUENTS: A,B

G(LIQUID,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +14000-10*T
G(LIQUID,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +18000-12*T
L(LIQUID,A,B;0) = 500.00<T< 2000.00: +V11+V12*T
L(LIQUID,A,B;1) = 500.00<T< 2000.00: +V13+V14*T

A2B
2 SUBLATTICES, SITES 2: 1
CONSTITUENTS: A : B

G(A2B,A;B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =
500.00<T< 2000.00: +V1+V2*T+V3*T*LN(T)

BCC
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
CONSTITUENTS: A,B

G(BCC,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +0.0
G(BCC,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +0.0
L(BCC,A,B;0) = 500.00<T< 2000.00: +V15+V16*T
L(BCC,A,B;1) = 500.00<T< 2000.00: +V17+V18*T

FCC
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
CONSTITUENTS: A,B

G(FCC,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +408
G(FCC,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +3300-3*T
L(FCC,A,B;0) = 500.00<T< 2000.00: +V19+V20*T
L(FCC,A,B;1) = 500.00<T< 2000.00: +V21+V22*T

$ ===== BLOCK NUMBER 1

```

```

DEFINED CONSTANTS
  DX=2E-2, P0=101325, DH=500, DT=10
DEFINED FUNCTIONS AND VARIABLES%
  HTR=HM(LIQUID)-HM(A2B)
1 T=1193                1192.        10.0        -1.201        -0.1201
1 W(LIQUID,B)=0.408      0.4083      2.00E-02    3.3615E-04    1.6807E-02
1 W(BCC,B)=0.13          0.1316      2.00E-02    1.5545E-03    7.7726E-02
2 T=1341                1342.        10.0        0.7529        7.5285E-02
2 HTR=3727              3678.        5.00E+02    -49.47        -9.8949E-02
3 T=1049                1047.        10.0        -1.645        -0.1645
3 W(LIQUID,A)=0.27       0.2711      2.00E-02    1.1266E-03    5.6332E-02
3 W(BCC,A)=9.3E-2       9.5336E-02   2.00E-02    2.3361E-03    0.1168
5 T=726                 724.5       10.0        -1.543        -0.1543
5 X(BCC,B)=3.7E-2       3.6647E-02   2.00E-02    -3.5272E-04   -1.7636E-02
5 X(BCC#2,A)=0.114      0.1147      2.00E-02    6.9816E-04    3.4908E-02
6 X(BCC,B)=3.7E-2       3.7082E-02   2.00E-02    8.1763E-05    4.0882E-03
6 X(BCC#2,A)=0.114      0.1158      2.00E-02    1.7838E-03    8.9192E-02
10 W(LIQUID,A)=2E-2      1.9559E-02   2.00E-02    -4.4094E-04   -2.2047E-02
11 W(LIQUID,A)=4.2E-2    4.1814E-02   2.00E-02    -1.8577E-04   -9.2884E-03
12 W(LIQUID,A)=6.5E-2    6.4837E-02   2.00E-02    -1.6291E-04   -8.1454E-03
13 W(LIQUID,A)=9.3E-2    9.2549E-02   2.00E-02    -4.5092E-04   -2.2546E-02
20 W(LIQUID,A)=0.104     0.1036      2.00E-02    -3.9164E-04   -1.9582E-02
20 W(FCC,A)=3.8E-2       3.8356E-02   2.00E-02    3.5602E-04    1.7801E-02
21 W(LIQUID,A)=0.136     0.1362      2.00E-02    1.9255E-04    9.6277E-03
21 W(FCC,A)=4.7E-2       4.7367E-02   2.00E-02    3.6734E-04    1.8367E-02
22 W(LIQUID,A)=0.187     0.1862      2.00E-02    -7.9799E-04   -3.9899E-02
22 W(FCC,A)=5.9E-2       5.9518E-02   2.00E-02    5.1760E-04    2.5880E-02
23 W(LIQUID,A)=0.245     0.2452      2.00E-02    1.8352E-04    9.1761E-03
23 W(BCC,A)=8.5E-2       8.6989E-02   2.00E-02    1.9894E-03    9.9469E-02

```

PARROT:

PARROT: @@ Note that all other experiments are well fitted!

PARROT: @@ Try to improve by optimizing a little more !!!

PARROT: resc

... the command in full is RESCALE\_VARIABLES

PARROT: opt 30

... the command in full is OPTIMIZE\_VARIABLES

Use 25 experiments, maximum is 2000

Use 494 real workspace, maximum is 50000

The following output is provided by subroutine VA05A

```

      AT THE      0 TH ITERATION WE HAVE THE SUM OF SQUARES      1.27916004E-01
1  1.0000E+00    2  1.0000E+00    3  1.0000E+00    4  1.0000E+00    5  1.0000E+00
6  1.0000E+00    7  1.0000E+00

      AT THE      1 ST ITERATION WE HAVE THE SUM OF SQUARES      1.27932261E-01
1  1.0001E+00    2  1.0000E+00    3  1.0000E+00    4  1.0000E+00    5  1.0000E+00
6  1.0000E+00    7  1.0000E+00

      AT THE      2 ND ITERATION WE HAVE THE SUM OF SQUARES      1.32349433E-01
1  1.0000E+00    2  1.0001E+00    3  1.0000E+00    4  1.0000E+00    5  1.0000E+00
6  1.0000E+00    7  1.0000E+00

      AT THE      3 RD ITERATION WE HAVE THE SUM OF SQUARES      1.27975279E-01
1  1.0000E+00    2  1.0000E+00    3  1.0001E+00    4  1.0000E+00    5  1.0000E+00
6  1.0000E+00    7  1.0000E+00

      AT THE      4 TH ITERATION WE HAVE THE SUM OF SQUARES      1.27918247E-01
1  1.0000E+00    2  1.0000E+00    3  1.0000E+00    4  1.0001E+00    5  1.0000E+00
6  1.0000E+00    7  1.0000E+00

      AT THE      5 TH ITERATION WE HAVE THE SUM OF SQUARES      1.27915991E-01
1  1.0000E+00    2  1.0000E+00    3  1.0000E+00    4  1.0000E+00    5  1.0001E+00
6  1.0000E+00    7  1.0000E+00

      AT THE      6 TH ITERATION WE HAVE THE SUM OF SQUARES      1.27919898E-01
1  1.0000E+00    2  1.0000E+00    3  1.0000E+00    4  1.0000E+00    5  1.0001E+00
6  1.0001E+00    7  1.0000E+00

      AT THE      7 TH ITERATION WE HAVE THE SUM OF SQUARES      1.27914900E-01
1  1.0000E+00    2  1.0000E+00    3  1.0000E+00    4  1.0000E+00    5  1.0001E+00
6  1.0000E+00    7  1.0001E+00

      AT THE      8 TH ITERATION WE HAVE THE SUM OF SQUARES      1.27686419E-01
1  1.0000E+00    2  9.9998E-01    3  1.0000E+00    4  1.0000E+00    5  1.0001E+00
6  1.0000E+00    7  1.0002E+00

      AT THE      9 TH ITERATION WE HAVE THE SUM OF SQUARES      1.27670632E-01
1  9.9993E-01    2  9.9993E-01    3  9.9998E-01    4  1.0000E+00    5  1.0001E+00
6  1.0001E+00    7  1.0002E+00

      THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED      9 iterations
1  9.9993E-01    2  9.9993E-01    3  9.9998E-01    4  1.0000E+00    5  1.0001E+00
6  1.0001E+00    7  1.0002E+00

1  -1.2292E-01    2  1.8762E-02    3  7.8915E-02    4  6.1120E-02    5  -9.7983E-02
6  -1.6559E-01    7  5.7097E-02    8  1.1773E-01    9  -1.5386E-01   10  -1.7437E-02
11  3.6109E-02   12  4.2281E-03   13  9.0250E-02   14  -2.1977E-02   15  -9.1582E-03
16  -7.9707E-03   17  -2.2338E-02   18  -1.9366E-02   19  1.8043E-02   20  9.8524E-03
21  1.8643E-02   22  -3.9695E-02   23  2.6185E-02   24  9.6601E-03   25  1.0017E-01

```

THE SUM OF SQUARES IS 1.27670632E-01

PARROT: l-r C SCREEN

... the command in full is LIST\_RESULT

```

=====
OUTPUT FROM P A R R O T.  DATE 2016. 5.16   14:21:50

```

\*\*\* SUCCESSFUL OPTIMIZATION. \*\*\*  
NUMBER OF ITERATIONS: 10

== OPTIMIZING CONDITIONS ==

```

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 30  DMAX = 1.00000000E+02  H = 1.00000000E-04

```

```

ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.   VALUE                START VALUE          SCALING FACTOR      REL.STAND.DEV
V1      2.04258378E+04        2.04272876E+04        2.04272876E+04      2.56056900E-02
V2      -2.95449125E+01       -2.95468613E+01       -2.95468613E+01      1.38446508E-02
V11     -2.18102047E+04        2.45250655E+04        2.45250655E+04      9.63618791E-02
V12      1.51613087E+01        2.45250655E+04        2.45250655E+04      2.70402366E-01
V15      2.45244730E+04        3.16252983E+03        3.16252983E+03      2.49505586E-01
V16     -8.85034461E+00       -8.85015072E+00       -8.85015072E+00      6.66481224E-01
V17      3.16285525E+03        2.20441098E+04        2.20441098E+04      1.56212011E+00
V19      2.20452445E+04        2.20441098E+04        2.20441098E+04      1.56212011E+00
V20     -7.16035825E+00       -7.15892220E+00       -7.15892220E+00      1.56212011E+00

NUMBER OF OPTIMIZING VARIABLES : 7
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 1.27916004E-01 TO 1.27670632E-01
DEGREES OF FREEDOM 18. REDUCED SUM OF SQUARES 7.09281289E-03

SYMBOL      STATUS  VALUE/FUNCTION
1 R          80000000 8.3145100E+00
2 RTLN      20000000 +R*T*LN(1E-05*P)
3 V1         48000000 2.0425838E+04
4 V2         48000000 -2.9544913E+01
13 V11       48000000 -2.1810205E+04
14 V12       48000000 1.5161309E+01
17 V15       48000000 2.4524473E+04
18 V16       48000000 -8.8503446E+00
19 V17       48000000 3.1628552E+03
21 V19       48000000 2.2045244E+04
22 V20       48000000 -7.1603583E+00

LIQUID
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
CONSTITUENTS: A,B

G(LIQUID,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +14000-10*T
G(LIQUID,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +18000-12*T
L(LIQUID,A,B;0) = 500.00<T< 2000.00: +V11+V12*T
L(LIQUID,A,B;1) = 500.00<T< 2000.00: +V13+V14*T

A2B
2 SUBLATTICES, SITES 2: 1
CONSTITUENTS: A : B

G(A2B,A;B;0) - 2 G(BCC,A;0) - G(BCC,B;0) =
500.00<T< 2000.00: +V1+V2*T+V3*T*LN(T)

BCC
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
CONSTITUENTS: A,B

G(BCC,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +0.0
G(BCC,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +0.0
L(BCC,A,B;0) = 500.00<T< 2000.00: +V15+V16*T
L(BCC,A,B;1) = 500.00<T< 2000.00: +V17+V18*T

FCC
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
CONSTITUENTS: A,B

G(FCC,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +408
G(FCC,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +3300-3*T
L(FCC,A,B;0) = 500.00<T< 2000.00: +V19+V20*T
L(FCC,A,B;1) = 500.00<T< 2000.00: +V21+V22*T

$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS
DX=2E-2, P0=101325, DH=500, DT=10
DEFINED FUNCTIONS AND VARIABLES%
HTR=HM(LIQUID)-HM(A2B)
1 T=1193 1192. 10.0 -1.229 -0.1229
1 W(LIQUID,B)=0.408 0.4084 2.00E-02 3.7523E-04 1.8762E-02
1 W(BCC,B)=0.13 0.1316 2.00E-02 1.5783E-03 7.8915E-02
2 T=1341 1342. 10.0 0.6112 6.1120E-02
2 HTR=3727 3678. 5.00E+02 -48.99 -9.7983E-02
3 T=1049 1047. 10.0 -1.656 -0.1656
3 W(LIQUID,A)=0.27 0.2711 2.00E-02 1.1419E-03 5.7097E-02
3 W(BCC,A)=9.3E-2 9.5355E-02 2.00E-02 2.3545E-03 0.1177
5 T=726 724.5 10.0 -1.539 -0.1539
5 X(BCC,B)=3.7E-2 3.6651E-02 2.00E-02 -3.4874E-04 -1.7437E-02
5 X(BCC#2,A)=0.114 0.1147 2.00E-02 7.2219E-04 3.6109E-02
6 X(BCC,B)=3.7E-2 3.7085E-02 2.00E-02 8.4561E-05 4.2281E-03
6 X(BCC#2,A)=0.114 0.1158 2.00E-02 1.8050E-03 9.0250E-02
10 W(LIQUID,A)=2E-2 1.9560E-02 2.00E-02 -4.3955E-04 -2.1977E-02
11 W(LIQUID,A)=4.2E-2 4.1817E-02 2.00E-02 -1.8316E-04 -9.1582E-03
12 W(LIQUID,A)=6.5E-2 6.4841E-02 2.00E-02 -1.5941E-04 -7.9707E-03
13 W(LIQUID,A)=9.3E-2 9.2553E-02 2.00E-02 -4.4677E-04 -2.2338E-02
20 W(LIQUID,A)=0.104 0.1036 2.00E-02 -3.8733E-04 -1.9366E-02
20 W(FCC,A)=3.8E-2 3.8361E-02 2.00E-02 3.6086E-04 1.8043E-02
21 W(LIQUID,A)=0.136 0.1362 2.00E-02 1.9705E-04 9.8524E-03
21 W(FCC,A)=4.7E-2 4.7373E-02 2.00E-02 3.7286E-04 1.8643E-02
22 W(LIQUID,A)=0.187 0.1862 2.00E-02 -7.9389E-04 -3.9695E-02
22 W(FCC,A)=5.9E-2 5.9524E-02 2.00E-02 5.2371E-04 2.6185E-02
23 W(LIQUID,A)=0.245 0.2452 2.00E-02 1.9320E-04 9.6601E-03
23 W(BCC,A)=8.5E-2 8.7003E-02 2.00E-02 2.0035E-03 0.1002

PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ Calculate the phase diagram again

```

```

PARROT: mac tcex36cpd
... the command in full is MACRO_FILE_OPEN
PARROT: set-echo
NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
... the command in full is GOTO_MODULE
POLY_3:
POLY_3: @@ In PARROT, the global minimization is turned off automatically.
POLY_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY_3: @@ message will be given.
POLY_3:
POLY_3: advanced-option global yes,,
... the command in full is ADVANCED_OPTIONS
Settings for global minimization:
*** WARNING *** Global equilibrium calculation may create new composition sets
and this may corrupt your PARROT work file (.PAR file).
Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY_3:
POLY_3: def-com,,,,
... the command in full is DEFINE_COMPONENTS
POLY_3: s-a-v 1 w(b) 0 1,,,,
... the command in full is SET_AXIS_VARIABLE
The condition W(B)=.1234 created
POLY_3: s-a-v 2 t 300 1700,,,,
... the command in full is SET_AXIS_VARIABLE
The condition T=942.2 created
POLY_3: s-c t=500
... the command in full is SET_CONDITION
POLY_3: l-c
... the command in full is LIST_CONDITIONS
W(B)=0.1234, P=1E5, N=1, T=500
DEGREES OF FREEDOM 0
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 412 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY_3: save tcex36 y
... the command in full is SAVE_WORKSPACES

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

POLY_3: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

Phase region boundary 1 at: 7.140E-01 3.100E+02
BCC
** BCC#2
Calculated.. 2 equilibria
Terminating at axis limit.

Phase region boundary 2 at: 7.141E-01 3.000E+02
BCC
** BCC#2
Calculated.. 14 equilibria

Phase region boundary 3 at: 6.813E-01 7.245E+02
** A2B
BCC
** BCC#2

Phase region boundary 4 at: 3.620E-01 7.245E+02
** A2B

```

```

      BCC
Calculated.                15 equilibria

Phase region boundary  5 at:  3.775E-01  1.192E+03
** LIQUID
** A2B
   BCC

Phase region boundary  6 at:  2.837E-01  1.192E+03
** LIQUID
   BCC
Calculated                26 equilibria

Phase region boundary  7 at:  4.865E-01  1.192E+03
** LIQUID
   A2B
Calculated.              33 equilibria

Phase region boundary  8 at:  6.495E-01  1.047E+03
** LIQUID
   A2B
** BCC

Phase region boundary  9 at:  7.626E-01  1.047E+03
   A2B
** BCC
Calculated.              11 equilibria
Terminating at known equilibrium

Phase region boundary 10 at:  8.258E-01  1.047E+03
   LIQUID
** BCC
Calculated.              9 equilibria

Phase region boundary 11 at:  8.763E-01  1.212E+03
   LIQUID
** BCC
** FCC

Phase region boundary 12 at:  8.820E-01  1.212E+03
   LIQUID
** FCC
Calculated              31 equilibria

Phase region boundary 13 at:  9.355E-01  1.212E+03
   BCC
** FCC
Calculated              23 equilibria

Phase region boundary 14 at:  7.140E-01  3.100E+02
   BCC
** BCC#2
Calculated.             13 equilibria
Terminating at known equilibrium

Phase region boundary 15 at:  7.140E-01  3.100E+02
   BCC
** BCC#2
Calculated..             2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 16 at:  7.140E-01  3.100E+02
   BCC
** BCC#2
Calculated.             13 equilibria
Terminating at known equilibrium

Phase region boundary 17 at:  7.140E-01  3.100E+02
   BCC
** BCC#2
Calculated..             2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 18 at:  7.140E-01  3.100E+02
   BCC
** BCC#2
Calculated.             13 equilibria
Terminating at known equilibrium

Phase region boundary 19 at:  7.140E-01  3.100E+02
   BCC
** BCC#2
Calculated..             2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 20 at:  7.140E-01  3.100E+02
   BCC
** BCC#2
Calculated.             13 equilibria
Terminating at known equilibrium

Phase region boundary 21 at:  7.140E-01  3.100E+02
** BCC
   BCC#2
Calculated..             2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 22 at:  7.140E-01  3.100E+02
** BCC
   BCC#2
Calculated.             13 equilibria
Terminating at known equilibrium

Phase region boundary 23 at:  7.140E-01  3.100E+02
** BCC
   BCC#2
Calculated..             2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 24 at:  7.140E-01  3.100E+02
** BCC

```

```

      BCC#2
Calculated.                13 equilibria
Terminating at known equilibrium

Phase region boundary 25 at: 3.642E-01 7.700E+02
** A2B
   BCC
Calculated                10 equilibria

Phase region boundary 26 at: 3.642E-01 7.700E+02
** A2B
   BCC
Calculated.                3 equilibria
Terminating at known equilibrium

Phase region boundary 27 at: 3.642E-01 7.700E+02
** A2B
   BCC
Calculated.                14 equilibria
Terminating at known equilibrium

Phase region boundary 28 at: 7.905E-01 7.700E+02
** A2B
   BCC
Calculated                10 equilibria

Phase region boundary 29 at: 7.905E-01 7.700E+02
** A2B
   BCC
Calculated.                3 equilibria
Terminating at known equilibrium

Phase region boundary 30 at: 7.905E-01 7.700E+02
** A2B
   BCC
Calculated.                9 equilibria
Terminating at known equilibrium

Phase region boundary 31 at: 2.451E-01 1.230E+03
** LIQUID
   BCC
Calculated.                4 equilibria
Terminating at known equilibrium

Phase region boundary 32 at: 2.451E-01 1.230E+03
** LIQUID
   BCC
Calculated                26 equilibria

Phase region boundary 33 at: 8.859E-01 1.230E+03
** LIQUID
   FCC
Calculated.                2 equilibria
Terminating at known equilibrium

Phase region boundary 34 at: 8.859E-01 1.230E+03
** LIQUID
   FCC
Calculated                29 equilibria

Phase region boundary 35 at: 6.428E-03 1.397E+03
   LIQUID
** BCC
Calculated                9 equilibria

Phase region boundary 36 at: 6.428E-03 1.397E+03
   LIQUID
** BCC
Calculated.                13 equilibria
Terminating at known equilibrium

Phase region boundary 37 at: 2.303E-01 1.244E+03
   LIQUID
** BCC
Calculated                21 equilibria

Phase region boundary 38 at: 2.303E-01 1.244E+03
   LIQUID
** BCC
Calculated.                4 equilibria
Terminating at known equilibrium

Phase region boundary 39 at: 6.122E-01 1.239E+03
   LIQUID
** A2B
Calculated.                14 equilibria
Terminating at known equilibrium

Phase region boundary 40 at: 6.122E-01 1.239E+03
   LIQUID
** A2B
Calculated.                8 equilibria
Terminating at known equilibrium

Phase region boundary 41 at: 9.927E-01 1.613E+03
   LIQUID
** FCC
Calculated.                19 equilibria
Terminating at known equilibrium

Phase region boundary 42 at: 9.927E-01 1.613E+03
   LIQUID
** FCC
Calculated                10 equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tce
x36.POLY3
CPU time for mapping                1 seconds
POLY_3: post
POST: s-l d
... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
... the command in full is PLOT_DIAGRAM

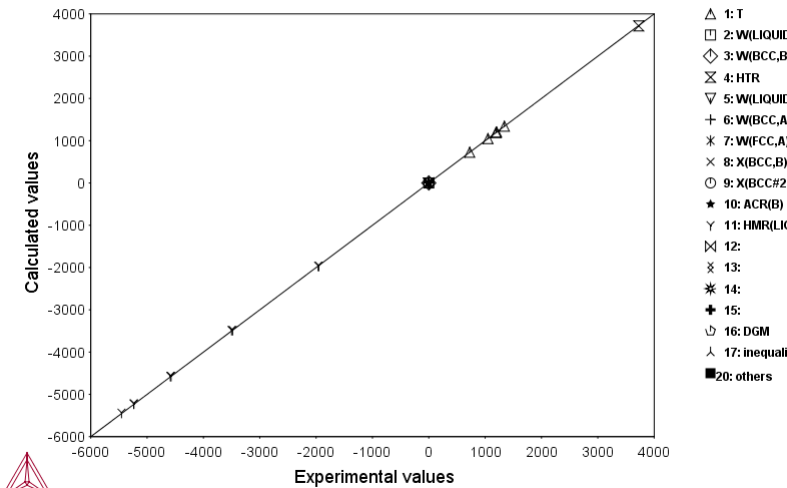
```

# From PARROT optimization

2016.05.16.14.21.54

A, B

P=1E5, N=1



POST:

POST: set-inter

... the command in full is SET\_INTERACTIVE\_MODE

POST: Hit RETURN to continue

POST: ba

... the command in full is BACK

POLY\_3: ba

... the command in full is BACK

PARROT VERSION 5.3

Global minimization used as test only

PARROT: @@ Now there is an equilibrium between fcc, bcc and liquid at high B

PARROT: @@ restore equilibrium 4 on the POP file

PARROT: ed

... the command in full is EDIT\_EXPERIMENTS

ED\_EXP: read 1

... the command in full is READ\_WORKSPACES

ED\_EXP: s-e 4

... the command in full is SELECT\_EQUILIBRIUM

Equilibrium number 4, label AINV

ED\_EXP: s-we 1

... the command in full is SET\_WEIGHT

Equilibria (range) or label(s) /PRESENT/: PRESENT

ED\_EXP: s-a-s

... the command in full is SET\_ALL\_START\_VALUES

T /1204.179217/: 1200

Automatic start values for phase constituents? /N/: N

Phase LIQUID

Major constituent(s) /b/: b

Phase BCC

Major constituent(s) /b/: b

Phase FCC

Major constituent(s) /b/: b

ED\_EXP:

ED\_EXP: c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Testing result with global minimization

13 ITS, CPU TIME USED 0 SECONDS

ED\_EXP: l-e

... the command in full is LIST\_EQUILIBRIUM

OUTPUT TO SCREEN OR FILE /SCREEN/:

Options /VWCS/: VWCS

Output from POLY-3, equilibrium = 4, label AINV, database:

Conditions:

P=1.01325E5

FIXED PHASES

LIQUID=1 BCC=1 FCC=1

DEGREES OF FREEDOM 0

Temperature 1211.86 K ( 938.71 C), Pressure 1.013250E+05

Number of moles of components 3.00000E+00, Mass in grams 1.30242E+02

Total Gibbs energy -1.00423E+04, Enthalpy 1.99596E+04, Volume 0.00000E+00

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
A	6.5861E-01	1.0114E-01	3.8286E-01	-9.6738E+03	SER
B	2.3414E+00	8.9886E-01	8.5590E-01	-1.5679E+03	SER

FCC	Status	FIXED	Driving force	0.0000E+00
Moles 1.0000E+00, Mass 4.5895E+01, Volume fraction 0.0000E+00	Mass fractions:			
B 9.40376E-01 A 5.96239E-02				

BCC	Status	FIXED	Driving force	0.0000E+00
Moles 1.0000E+00, Mass 4.5283E+01, Volume fraction 0.0000E+00	Mass fractions:			
B 9.30557E-01 A 6.94426E-02				

LIQUID	Status	FIXED	Driving force	0.0000E+00
Moles 1.0000E+00, Mass 3.9063E+01, Volume fraction 0.0000E+00	Mass fractions:			
B 8.13351E-01 A 1.86649E-01				

EXPERIMENT T=1203:DT \$1211.86:10 NO=1

EXPERIMENT W(LIQUID,A)=0.19:DX \$0.186649:2E-2 NO=2

EXPERIMENT W(BCC,A)=6.9E-2:DX \$6.94426E-2:2E-2 NO=3

EXPERIMENT W(FCC,A)=6E-2:DX \$5.96239E-2:2E-2 NO=4

ED\_EXP: @@ Now equilibrium 4 is on the high B side

ED\_EXP: save

... the command in full is SAVE\_WORKSPACES

```
ED_EXP: ba
... the command in full is BACK
PARROT: resc
... the command in full is RESCALE_VARIABLES
PARROT: opt 0
... the command in full is OPTIMIZE_VARIABLES
Use      29 experiments, maximum is      2000
Use      554 real workspace, maximum is    50000
PARROT: l-r C SCREEN
... the command in full is LIST_RESULT
```

```
=====
OUTPUT FROM P A R R O T.  DATE 2016. 5.16   14:21:55
```

```
*** SUCCESSFUL OPTIMIZATION. ***
NUMBER OF ITERATIONS: 0
```

```
== OPTIMIZING CONDITIONS ==
```

```
RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N
MINIMUM SAVE ON FILE: Y
ERROR FOR INEQUALITIES = 1.00000000E+00
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)
MAXFUN = 0 DMAX = 1.00000000E+02 H = 1.00000000E-04
ACC = (INITIAL SUM OF SQUARES) * 1.00000000E-03
```

```
== OPTIMIZING VARIABLES ==
```

```
AVAILABLE VARIABLES ARE V1 TO V00
```

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.04258378E+04	2.04258378E+04	2.04258378E+04	0.00000000E+00
V2	-2.95449125E+01	-2.95449125E+01	-2.95449125E+01	0.00000000E+00
V11	-2.18102047E+04			
V12	1.51613087E+01			
V15	2.45244730E+04	2.45244730E+04	2.45244730E+04	0.00000000E+00
V16	-8.85034461E+00	-8.85034461E+00	-8.85034461E+00	0.00000000E+00
V17	3.16285525E+03	3.16285525E+03	3.16285525E+03	0.00000000E+00
V19	2.20452445E+04	2.20452445E+04	2.20452445E+04	0.00000000E+00
V20	-7.16035825E+00	-7.16035825E+00	-7.16035825E+00	0.00000000E+00

```
NUMBER OF OPTIMIZING VARIABLES : 7
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 0.00000000E+00 TO 9.41736381E-01
DEGREES OF FREEDOM 22. REDUCED SUM OF SQUARES 4.28061991E-02
```

SYMBOL	STATUS	VALUE/FUNCTION
1 R	80000000	8.3145100E+00
2 RTLN	20000000	+R*T*LN(1E-05*P)
3 V1	48000000	2.0425838E+04
4 V2	48000000	-2.9544913E+01
13 V11	48000000	-2.1810205E+04
14 V12	48000000	1.5161309E+01
17 V15	48000000	2.4524473E+04
18 V16	48000000	-8.8503446E+00
19 V17	48000000	3.1628552E+03
21 V19	48000000	2.2045244E+04
22 V20	48000000	-7.1603583E+00

```
LIQUID
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
CONSTITUENTS: A,B
```

```
G(LIQUID,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +14000-10*T
G(LIQUID,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +18000-12*T
L(LIQUID,A,B;0) = 500.00<T< 2000.00: +V11+V12*T
L(LIQUID,A,B;1) = 500.00<T< 2000.00: +V13+V14*T
```

```
A2B
2 SUBLATTICES, SITES 2: 1
CONSTITUENTS: A : B
```

```
G(A2B,A;B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =
500.00<T< 2000.00: +V1+V2*T+V3*T*LN(T)
```

```
BCC
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
CONSTITUENTS: A,B
```

```
G(BCC,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +0.0
G(BCC,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +0.0
L(BCC,A,B;0) = 500.00<T< 2000.00: +V15+V16*T
L(BCC,A,B;1) = 500.00<T< 2000.00: +V17+V18*T
```

```
FCC
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
CONSTITUENTS: A,B
```

```
G(FCC,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +408
G(FCC,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +3300-3*T
L(FCC,A,B;0) = 500.00<T< 2000.00: +V19+V20*T
L(FCC,A,B;1) = 500.00<T< 2000.00: +V21+V22*T
```

```
$ ===== BLOCK NUMBER 1
```

```
DEFINED CONSTANTS
DX=2E-2, P0=101325, DH=500, DT=10
DEFINED FUNCTIONS AND VARIABLES%
HTR=HM(LIQUID)-HM(A2B)
```



```

1 T=1193 1192. 10.0 -1.229 -0.1229
1 W(LIQUID,B)=0.408 0.4084 2.00E-02 3.7523E-04 1.8762E-02
1 W(BCC,B)=0.13 0.1316 2.00E-02 1.5783E-03 7.8915E-02
2 T=1341 1342. 10.0 0.6112 6.1120E-02
2 HTR=3727 3678. 5.00E+02 -48.99 -9.7983E-02
3 T=1049 1047. 10.0 -1.656 -0.1656
3 W(LIQUID,A)=0.27 0.2711 2.00E-02 1.1419E-03 5.7097E-02
3 W(BCC,A)=9.3E-2 9.5355E-02 2.00E-02 2.3545E-03 0.1177
4 T=1203 1212. 10.0 8.861 0.8861
4 W(LIQUID,A)=0.19 0.1866 2.00E-02 -3.3513E-03 -0.1676
4 W(BCC,A)=6.9E-2 6.9443E-02 2.00E-02 4.4257E-04 2.2128E-02
4 W(FCC,A)=6E-2 5.9624E-02 2.00E-02 -3.7607E-04 -1.8803E-02
5 T=726 724.5 10.0 -1.539 -0.1539
5 X(BCC,B)=3.7E-2 3.6651E-02 2.00E-02 -3.4874E-04 -1.7437E-02
5 X(BCC#2,A)=0.114 0.1147 2.00E-02 7.2219E-04 3.6109E-02
6 X(BCC,B)=3.7E-2 3.7085E-02 2.00E-02 8.4561E-05 4.2281E-03
6 X(BCC#2,A)=0.114 0.1158 2.00E-02 1.8050E-03 9.0250E-02
10 W(LIQUID,A)=2E-2 1.9560E-02 2.00E-02 -4.3955E-04 -2.1977E-02
11 W(LIQUID,A)=4.2E-2 4.1817E-02 2.00E-02 -1.8316E-04 -9.1582E-03
12 W(LIQUID,A)=6.5E-2 6.4841E-02 2.00E-02 -1.5941E-04 -7.9707E-03
13 W(LIQUID,A)=9.3E-2 9.2553E-02 2.00E-02 -4.4677E-04 -2.2338E-02
20 W(LIQUID,A)=0.104 0.1036 2.00E-02 -3.8733E-04 -1.9366E-02
20 W(FCC,A)=3.8E-2 3.8361E-02 2.00E-02 3.6086E-04 1.8043E-02
21 W(LIQUID,A)=0.136 0.1362 2.00E-02 1.9705E-04 9.8524E-03
21 W(FCC,A)=4.7E-2 4.7373E-02 2.00E-02 3.7286E-04 1.8643E-02
22 W(LIQUID,A)=0.187 0.1862 2.00E-02 -7.9389E-04 -3.9695E-02
22 W(FCC,A)=5.9E-2 5.9524E-02 2.00E-02 5.2371E-04 2.6185E-02
23 W(LIQUID,A)=0.245 2.2452 2.00E-02 1.9320E-04 9.6601E-03
23 W(BCC,A)=8.5E-2 8.7003E-02 2.00E-02 2.0035E-03 0.1002

```

PARROT:  
PARROT:Hit RETURN to continue

PARROT: opt 30  
... the command in full is OPTIMIZE\_VARIABLES  
Use 29 experiments, maximum is 2000  
Use 554 real workspace, maximum is 50000  
The following output is provided by subroutine VA05A

```

      AT THE      0 TH ITERATION WE HAVE THE SUM OF SQUARES      9.41736381E-01
1  1.0000E+00      2  1.0000E+00      3  1.0000E+00      4  1.0000E+00      5  1.0000E+00
6  1.0000E+00      7  1.0000E+00

      AT THE      1 ST ITERATION WE HAVE THE SUM OF SQUARES      9.42553951E-01
1  1.0001E+00      2  1.0000E+00      3  1.0000E+00      4  1.0000E+00      5  1.0000E+00
6  1.0000E+00      7  1.0000E+00

      AT THE      2 ND ITERATION WE HAVE THE SUM OF SQUARES      9.44643142E-01
1  1.0000E+00      2  1.0001E+00      3  1.0000E+00      4  1.0000E+00      5  1.0000E+00
6  1.0000E+00      7  1.0000E+00

      AT THE      3 RD ITERATION WE HAVE THE SUM OF SQUARES      9.18434003E-01
1  1.0000E+00      2  1.0000E+00      3  1.0001E+00      4  1.0000E+00      5  1.0000E+00
6  1.0000E+00      7  1.0000E+00

      AT THE      4 TH ITERATION WE HAVE THE SUM OF SQUARES      9.28574725E-01
1  1.0000E+00      2  1.0000E+00      3  1.0001E+00      4  1.0001E+00      5  1.0000E+00
6  1.0000E+00      7  1.0000E+00

      AT THE      5 TH ITERATION WE HAVE THE SUM OF SQUARES      9.20479911E-01
1  1.0000E+00      2  1.0000E+00      3  1.0001E+00      4  1.0000E+00      5  1.0001E+00
6  1.0000E+00      7  1.0000E+00

      AT THE      6 TH ITERATION WE HAVE THE SUM OF SQUARES      9.35680621E-01
1  1.0000E+00      2  1.0000E+00      3  1.0001E+00      4  1.0000E+00      5  1.0000E+00
6  1.0001E+00      7  1.0000E+00

      AT THE      7 TH ITERATION WE HAVE THE SUM OF SQUARES      9.11696096E-01
1  1.0000E+00      2  1.0000E+00      3  1.0001E+00      4  1.0000E+00      5  1.0000E+00
6  1.0000E+00      7  1.0001E+00

      AT THE      8 TH ITERATION WE HAVE THE SUM OF SQUARES      2.18168252E-01
1  1.0000E+00      2  9.9999E-01      3  1.0034E+00      4  9.9857E-01      5  9.9971E-01
6  9.9757E-01      7  1.0011E+00

      AT THE      9 TH ITERATION WE HAVE THE SUM OF SQUARES      2.07235143E-01
1  9.9990E-01      2  1.0000E+00      3  1.0024E+00      4  9.9680E-01      5  9.9848E-01
6  9.9610E-01      7  9.9760E-01

      AT THE     10 TH ITERATION WE HAVE THE SUM OF SQUARES      1.87994192E-01
1  9.9973E-01      2  9.9985E-01      3  1.0004E+00      4  9.9280E-01      5  9.9574E-01
6  9.9339E-01      7  9.9099E-01

      AT THE     11 TH ITERATION WE HAVE THE SUM OF SQUARES      1.62151889E-01
1  9.9932E-01      2  9.9968E-01      3  9.9655E-01      4  9.8495E-01      5  9.9036E-01
6  9.8792E-01      7  9.7763E-01

      AT THE     12 TH ITERATION WE HAVE THE SUM OF SQUARES      1.50053570E-01
1  9.9877E-01      2  9.9938E-01      3  9.9141E-01      4  9.7448E-01      5  9.8315E-01
6  9.8103E-01      7  9.6066E-01

THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED      12 iterations
1  9.9877E-01      2  9.9938E-01      3  9.9141E-01      4  9.7448E-01      5  9.8315E-01
6  9.8103E-01      7  9.6066E-01

1 -1.1651E-01      2  1.0617E-02      3  6.2552E-02      4  6.6364E-02      5 -8.1216E-02
6 -2.1958E-01      7  4.1235E-02      8  8.3058E-02      9  2.9863E-02     10  2.5417E-02
11  4.5304E-02     12  5.9829E-02     13 -1.7379E-01     14  1.8247E-02     15  4.5330E-02
16  4.3059E-02     17  1.0640E-01     18 -2.3843E-02     19 -1.1306E-02     20 -8.6872E-03
21 -1.9428E-02     22 -1.4518E-02     23  2.3484E-02     24  2.1765E-02     25  3.3281E-02
26 -1.3748E-02     27  6.4932E-02     28 -2.4111E-02     29  5.6807E-02

```

THE SUM OF SQUARES IS 1.50053570E-01  
PARROT: l-r C SCREEN  
... the command in full is LIST\_RESULT

=====

OUTPUT FROM P A R R O T. DATE 2016. 5.16 14:21:56

\*\*\* SUCCESSFUL OPTIMIZATION. \*\*\*  
NUMBER OF ITERATIONS: 13

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N  
MINIMUM SAVE ON FILE: Y  
ERROR FOR INEQUALITIES = 1.00000000E+00  
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04  
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)  
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04  
ACC = (INITIAL SUM OF SQUARES) \* 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.04006875E+04	2.04258378E+04	2.04258378E+04	2.41616566E-02
V2	-2.95264884E+01	-2.95449125E+01	-2.95449125E+01	1.31557074E-02
V11	-2.18102047E+04			
V12	1.51613087E+01			
V15	2.43137486E+04	2.45244730E+04	2.45244730E+04	7.66766133E-02
V16	-8.62447823E+00	-8.85034461E+00	-8.85034461E+00	2.08107836E-01
V17	3.10957097E+03	3.16285525E+03	3.16285525E+03	2.22191980E-01
V19	2.16271390E+04	2.20452445E+04	2.20452445E+04	4.98933483E-01
V20	-6.87864884E+00	-7.16035825E+00	-7.16035825E+00	1.22727290E+00

NUMBER OF OPTIMIZING VARIABLES : 7  
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO  
THE SUM OF SQUARES HAS CHANGED FROM 9.41736381E-01 TO 1.50053570E-01  
DEGREES OF FREEDOM 22. REDUCED SUM OF SQUARES 6.82061684E-03

SYMBOL	STATUS	VALUE/FUNCTION
1 R	80000000	8.3145100E+00
2 RTLNP	20000000	+R*T*LN(1E-05*P)
3 V1	48000000	2.0400688E+04
4 V2	48000000	-2.9526488E+01
13 V11	48000000	-2.1810205E+04
14 V12	48000000	1.5161309E+01
17 V15	48000000	2.4313749E+04
18 V16	48000000	-8.6244782E+00
19 V17	48000000	3.1095710E+03
21 V19	48000000	2.1627139E+04
22 V20	48000000	-6.8786488E+00

LIQUID  
EXCESS MODEL IS REDLICH-KISTER\_MUGGIANU  
CONSTITUENTS: A,B

G(LIQUID,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +14000-10\*T  
G(LIQUID,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +18000-12\*T  
L(LIQUID,A,B;0) = 500.00<T< 2000.00: +V11+V12\*T  
L(LIQUID,A,B;1) = 500.00<T< 2000.00: +V13+V14\*T

A2B  
2 SUBLATTICES, SITES 2: 1  
CONSTITUENTS: A : B

G(A2B,A;B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =  
500.00<T< 2000.00: +V1+V2\*T+V3\*T\*LN(T)

BCC  
EXCESS MODEL IS REDLICH-KISTER\_MUGGIANU  
CONSTITUENTS: A,B

G(BCC,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +0.0  
G(BCC,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +0.0  
L(BCC,A,B;0) = 500.00<T< 2000.00: +V15+V16\*T  
L(BCC,A,B;1) = 500.00<T< 2000.00: +V17+V18\*T

FCC  
EXCESS MODEL IS REDLICH-KISTER\_MUGGIANU  
CONSTITUENTS: A,B

G(FCC,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +408  
G(FCC,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +3300-3\*T  
L(FCC,A,B;0) = 500.00<T< 2000.00: +V19+V20\*T  
L(FCC,A,B;1) = 500.00<T< 2000.00: +V21+V22\*T

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS

DX=2E-2, P0=101325, DH=500, DT=10

DEFINED FUNCTIONS AND VARIABLES%

HTR=HM(LIQUID)-HM(A2B)

1 T=1193	1192.	10.0	-1.165	-0.1165
1 W(LIQUID,B)=0.408	0.4082	2.00E-02	2.1234E-04	1.0617E-02
1 W(BCC,B)=0.13	0.1313	2.00E-02	1.2510E-03	6.2552E-02
2 T=1341	1342.	10.0	0.6636	6.6364E-02
2 HTR=3727	3686.	5.00E+02	-40.61	-8.1216E-02
3 T=1049	1047.	10.0	-2.196	-0.2196
3 W(LIQUID,A)=0.27	0.2708	2.00E-02	8.2469E-04	4.1235E-02
3 W(BCC,A)=9.3E-2	9.4661E-02	2.00E-02	1.6612E-03	8.3058E-02
4 T=1203	1203.	10.0	0.2986	2.9863E-02
4 W(LIQUID,A)=0.19	0.1905	2.00E-02	5.0833E-04	2.5417E-02
4 W(BCC,A)=6.9E-2	6.9906E-02	2.00E-02	9.0608E-04	4.5304E-02
4 W(FCC,A)=6E-2	6.1197E-02	2.00E-02	1.1966E-03	5.9829E-02
5 T=726	724.3	10.0	-1.738	-0.1738
5 X(BCC,B)=3.7E-2	3.7365E-02	2.00E-02	3.6493E-04	1.8247E-02
5 X(BCC#2,A)=0.114	0.1149	2.00E-02	9.0661E-04	4.5330E-02
6 X(BCC,B)=3.7E-2	3.7861E-02	2.00E-02	8.6118E-04	4.3059E-02
6 X(BCC#2,A)=0.114	0.1161	2.00E-02	2.1279E-03	0.1064
10 W(LIQUID,A)=2E-2	1.9523E-02	2.00E-02	-4.7686E-04	-2.3843E-02
11 W(LIQUID,A)=4.2E-2	4.1774E-02	2.00E-02	-2.2612E-04	-1.1306E-02
12 W(LIQUID,A)=6.5E-2	6.4826E-02	2.00E-02	-1.7374E-04	-8.6872E-03

```

13 W(LIQUID,A)=9.3E-2          9.2611E-02  2.00E-02 -3.8856E-04 -1.9428E-02
20 W(LIQUID,A)=0.104          0.1037      2.00E-02 -2.9035E-04 -1.4518E-02
20 W(FCC,A)=3.8E-2            3.8470E-02  2.00E-02  4.6968E-04  2.3484E-02
21 W(LIQUID,A)=0.136          0.1364      2.00E-02  4.3530E-04  2.1765E-02
21 W(FCC,A)=4.7E-2            4.7666E-02  2.00E-02  6.6563E-04  3.3281E-02
22 W(LIQUID,A)=0.187          0.1867      2.00E-02 -2.7497E-04 -1.3748E-02
22 W(FCC,A)=5.9E-2            6.0299E-02  2.00E-02  1.2986E-03  6.4932E-02
23 W(LIQUID,A)=0.245          0.2445      2.00E-02 -4.8222E-04 -2.4111E-02
23 W(BCC,A)=8.5E-2            8.6136E-02  2.00E-02  1.1361E-03  5.6807E-02

```

```

PARROT:
PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ Now optimize all parameters and all experiments
PARROT: l-a-v
... the command in full is LIST_ALL_VARIABLES
OUTPUT TO SCREEN OR FILE /SCREEN/:

```

```
== OPTIMIZING VARIABLES ==
```

```
AVAILABLE VARIABLES ARE V1 TO V00
```

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.04006875E+04	2.04258378E+04	2.04258378E+04	2.41616566E-02
V2	-2.95264884E+01	-2.95449125E+01	-2.95449125E+01	1.31557074E-02
V11	-2.18102047E+04			
V12	1.51613087E+01			
V15	2.43137486E+04	2.45244730E+04	2.45244730E+04	7.66766133E-02
V16	-8.62447823E+00	-8.85034461E+00	-8.85034461E+00	2.08107836E-01
V17	3.10957097E+03	3.16285525E+03	3.16285525E+03	2.22191980E-01
V19	2.16271390E+04	2.20452445E+04	2.20452445E+04	4.98933483E-01
V20	-6.87864884E+00	-7.16035825E+00	-7.16035825E+00	1.22727290E+00

```

NUMBER OF OPTIMIZING VARIABLES : 7
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO
THE SUM OF SQUARES HAS CHANGED FROM 9.41736381E-01 TO 1.50053570E-01
DEGREES OF FREEDOM 22. REDUCED SUM OF SQUARES 6.82061684E-03

```

```

PARROT: s-o-v 11-12
... the command in full is SET_OPTIMIZING_VARIABLE
PARROT: ed
... the command in full is EDIT_EXPERIMENTS

```

```

ED_EXP: read 1
... the command in full is READ_WORKSPACES
ED_EXP: c-a
... the command in full is COMPUTE_ALL_EQUILIBRIA

```

Eq	Lab	Iter	Weight	Temp	Exp	Fix phases or comments
1	AINV	2	1.	1191.8		LIQUID A2B BCC
2	AINV	2	1.	1341.7		LIQUID A2B
3	AINV	2	1.	1046.8		LIQUID A2B BCC
4	AINV	2	1.	1203.3		LIQUID BCC FCC
5	AINV	2	1.	724.3		A2B BCC BCC#2
6	AINV	2	1.	726.0		BCC BCC#2
10	ALF	2	1.	1594.0		LIQUID FCC
11	ALF	2	1.	1548.0		LIQUID FCC
12	ALF	2	1.	1499.0		LIQUID FCC
13	ALF	2	1.	1438.0		LIQUID FCC
20	ATIE	2	1.	1413.0		LIQUID FCC
21	ATIE	2	1.	1337.0		LIQUID FCC
22	ATIE	2	1.	1213.0		LIQUID FCC
23	ATIE	2	1.	1100.0		LIQUID BCC
100	AA	< unused >		1573.0		LIQUID
101	AA	< unused >		1573.0		LIQUID
102	AA	< unused >		1573.0		LIQUID
103	AA	< unused >		1573.0		LIQUID
104	AA	< unused >		1573.0		LIQUID
105	AA	< unused >		1573.0		LIQUID
106	AA	< unused >		1573.0		LIQUID
107	AA	< unused >		1573.0		LIQUID
108	AA	< unused >		1573.0		LIQUID
110	AH	< unused >		1773.0		LIQUID
111	AH	< unused >		1773.0		LIQUID
112	AH	< unused >		1773.0		LIQUID
113	AH	< unused >		1773.0		LIQUID
114	AH	< unused >		1773.0		LIQUID
115	AH	< unused >		1773.0		LIQUID
116	AH	< unused >		1773.0		LIQUID
117	AH	< unused >		1773.0		LIQUID
118	AH	< unused >		1773.0		LIQUID

```

ED_EXP: s-we 1 100-118
... the command in full is SET_WEIGHT
ED_EXP: s-e 1
... the command in full is SELECT_EQUILIBRIUM

```

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

... the command in full is SAVE\_WORKSPACES

ED\_EXP: ba

... the command in full is BACK

PARROT: opt 30

... the command in full is OPTIMIZE\_VARIABLES

Use 47 experiments, maximum is 2000

Use 1082 real workspace, maximum is 50000

The following output is provided by subroutine VA05A

```
      AT THE      0 TH ITERATION WE HAVE THE SUM OF SQUARES      1.71348983E-01
1  9.9877E-01      2  9.9938E-01      3  1.0000E+00      4  1.0000E+00      5  9.9141E-01
6  9.7448E-01      7  9.8315E-01      8  9.8103E-01      9  9.6066E-01
```

```
      AT THE      1 ST ITERATION WE HAVE THE SUM OF SQUARES      1.72203930E-01
1  9.9887E-01      2  9.9938E-01      3  1.0000E+00      4  1.0000E+00      5  9.9141E-01
6  9.7448E-01      7  9.8315E-01      8  9.8103E-01      9  9.6066E-01
```

```
      AT THE      2 ND ITERATION WE HAVE THE SUM OF SQUARES      1.74167084E-01
1  9.9877E-01      2  9.9948E-01      3  1.0000E+00      4  1.0000E+00      5  9.9141E-01
6  9.7448E-01      7  9.8315E-01      8  9.8103E-01      9  9.6066E-01
```

```
      AT THE      3 RD ITERATION WE HAVE THE SUM OF SQUARES      1.75634356E-01
1  9.9877E-01      2  9.9938E-01      3  1.0001E+00      4  1.0000E+00      5  9.9141E-01
6  9.7448E-01      7  9.8315E-01      8  9.8103E-01      9  9.6066E-01
```

```
      AT THE      4 TH ITERATION WE HAVE THE SUM OF SQUARES      1.69474652E-01
1  9.9877E-01      2  9.9938E-01      3  1.0000E+00      4  1.0001E+00      5  9.9141E-01
6  9.7448E-01      7  9.8315E-01      8  9.8103E-01      9  9.6066E-01
```

```
      AT THE      5 TH ITERATION WE HAVE THE SUM OF SQUARES      1.69562798E-01
1  9.9877E-01      2  9.9938E-01      3  1.0000E+00      4  1.0001E+00      5  9.9151E-01
6  9.7448E-01      7  9.8315E-01      8  9.8103E-01      9  9.6066E-01
```

```
      AT THE      6 TH ITERATION WE HAVE THE SUM OF SQUARES      1.69566267E-01
1  9.9877E-01      2  9.9938E-01      3  1.0000E+00      4  1.0001E+00      5  9.9141E-01
6  9.7458E-01      7  9.8315E-01      8  9.8103E-01      9  9.6066E-01
```

```
      AT THE      7 TH ITERATION WE HAVE THE SUM OF SQUARES      1.69484800E-01
1  9.9877E-01      2  9.9938E-01      3  1.0000E+00      4  1.0001E+00      5  9.9141E-01
6  9.7448E-01      7  9.8325E-01      8  9.8103E-01      9  9.6066E-01
```

```
      AT THE      8 TH ITERATION WE HAVE THE SUM OF SQUARES      1.69600694E-01
1  9.9877E-01      2  9.9938E-01      3  1.0000E+00      4  1.0001E+00      5  9.9141E-01
6  9.7448E-01      7  9.8315E-01      8  9.8113E-01      9  9.6066E-01
```

```
      AT THE      9 TH ITERATION WE HAVE THE SUM OF SQUARES      1.69486726E-01
1  9.9877E-01      2  9.9938E-01      3  1.0000E+00      4  1.0001E+00      5  9.9141E-01
6  9.7448E-01      7  9.8315E-01      8  9.8103E-01      9  9.6076E-01
```

```
      AT THE     10 TH ITERATION WE HAVE THE SUM OF SQUARES      1.52786177E-01
1  9.9900E-01      2  9.9895E-01      3  9.9938E-01      4  1.0004E+00      5  9.9144E-01
6  9.7447E-01      7  9.8315E-01      8  9.8103E-01      9  9.6066E-01
```

```
      AT THE     11 TH ITERATION WE HAVE THE SUM OF SQUARES      1.40532739E-01
1  9.9890E-01      2  9.9900E-01      3  9.9926E-01      4  1.0005E+00      5  9.9136E-01
6  9.7393E-01      7  9.8302E-01      8  9.8140E-01      9  9.6114E-01
```

```
      AT THE     12 TH ITERATION WE HAVE THE SUM OF SQUARES      1.29724490E-01
1  9.9893E-01      2  9.9866E-01      3  9.9885E-01      4  1.0007E+00      5  9.9142E-01
6  9.7290E-01      7  9.8276E-01      8  9.8209E-01      9  9.6210E-01
```

```
      AT THE     13 TH ITERATION WE HAVE THE SUM OF SQUARES      1.15934436E-01
1  9.9874E-01      2  9.9848E-01      3  9.9859E-01      4  1.0010E+00      5  9.9102E-01
6  9.7065E-01      7  9.8221E-01      8  9.8360E-01      9  9.6396E-01
```

```
      AT THE     14 TH ITERATION WE HAVE THE SUM OF SQUARES      9.75379513E-02
1  9.9849E-01      2  9.9788E-01      3  9.9801E-01      4  1.0015E+00      5  9.9032E-01
6  9.6628E-01      7  9.8112E-01      8  9.8668E-01      9  9.6777E-01
```

```
      AT THE     15 TH ITERATION WE HAVE THE SUM OF SQUARES      7.50720931E-02
1  9.9786E-01      2  9.9702E-01      3  9.9725E-01      4  1.0024E+00      5  9.8867E-01
6  9.5729E-01      7  9.7889E-01      8  9.9265E-01      9  9.7533E-01
```

```
      AT THE     16 TH ITERATION WE HAVE THE SUM OF SQUARES      6.73903735E-02
1  9.9721E-01      2  9.9606E-01      3  9.9646E-01      4  1.0033E+00      5  9.8691E-01
6  9.4769E-01      7  9.7652E-01      8  9.9896E-01      9  9.8321E-01
```

```
THE FINAL SOLUTION CALCULATED BY VA05A REQUIRED      16 iterations
1  9.9721E-01      2  9.9606E-01      3  9.9646E-01      4  1.0033E+00      5  9.8691E-01
6  9.4769E-01      7  9.7652E-01      8  9.9896E-01      9  9.8321E-01
```

```
1 -5.7769E-02      2 -9.3761E-03      3  1.4158E-02      4  2.0690E-02      5 -2.5688E-02
6 -5.1171E-02      7  1.9343E-02      8  2.7056E-02      9  1.2439E-02     10  2.7688E-02
11 9.1632E-03     12  1.3813E-02     13 -4.8791E-02     14  2.1460E-02     15  4.7007E-03
16 2.8358E-02     17  2.1568E-02     18 -2.2454E-02     19 -8.9460E-03     20 -5.8150E-03
21 -1.6458E-02     22 -1.1654E-02     23  1.4345E-02     24  2.3824E-02     25  1.4109E-02
26 -1.4553E-02     27  2.0708E-02     28 -1.2425E-02     29  1.5727E-02     30 -9.5825E-03
31 -1.6802E-02     32  2.7496E-02     33  8.7112E-02     34  1.2446E-01     35  1.0182E-01
36 -1.7174E-02     37  7.0704E-02     38 -1.9397E-02     39  1.6052E-02     40  4.5425E-02
41 4.8120E-02     42  4.6137E-02     43  4.1476E-02     44  3.4137E-02     45  2.2120E-02
46 7.4249E-03     47 -1.1948E-02
```

THE SUM OF SQUARES IS 6.73903735E-02

PARROT: l-r C SCREEN

... the command in full is LIST\_RESULT

```
=====
OUTPUT FROM  P A R R O T.  DATE 2016. 5.16   14:21:56
```

\*\*\* SUCCESSFUL OPTIMIZATION. \*\*\*  
NUMBER OF ITERATIONS: 17

== OPTIMIZING CONDITIONS ==

RELATIVE STANDARD DEVIATIONS FOR EXPERIMENTS: N

MINIMUM SAVE ON FILE: Y  
ERROR FOR INEQUALITIES = 1.00000000E+00  
RELATIVE STEP FOR CALCULATION OF DERIVATIVES = 1.00000000E-04  
ARGUMENTS FOR SUBROUTINE VA05AD (HSL)  
MAXFUN = 30 DMAX = 1.00000000E+02 H = 1.00000000E-04  
ACC = (INITIAL SUM OF SQUARES) \* 1.00000000E-03

== OPTIMIZING VARIABLES ==

AVAILABLE VARIABLES ARE V1 TO V00

VAR.	VALUE	START VALUE	SCALING FACTOR	REL.STAND.DEV
V1	2.03688341E+04	2.04258378E+04	2.04258378E+04	2.96135417E-02
V2	-2.94286301E+01	-2.95449125E+01	-2.95449125E+01	2.25274567E-02
V11	-2.17330472E+04	-2.18102047E+04	-2.18102047E+04	3.47407502E-02
V12	1.52107324E+01	1.51613087E+01	1.51613087E+01	5.56505566E-02
V15	2.42035190E+04	2.45244730E+04	2.45244730E+04	8.09093794E-02
V16	-8.38741946E+00	-8.85034461E+00	-8.85034461E+00	2.37193886E-01
V17	3.08858371E+03	3.16285525E+03	3.16285525E+03	2.23457303E-01
V19	2.20222843E+04	2.20452445E+04	2.20452445E+04	4.94492773E-01
V20	-7.04010396E+00	-7.16035825E+00	-7.16035825E+00	1.21662443E+00

NUMBER OF OPTIMIZING VARIABLES : 9  
ALL OTHER VARIABLES ARE FIX WITH THE VALUE ZERO  
THE SUM OF SQUARES HAS CHANGED FROM 1.71348983E-01 TO 6.73903735E-02  
DEGREES OF FREEDOM 38. REDUCED SUM OF SQUARES 1.77343088E-03

SYMBOL	STATUS	VALUE/FUNCTION
1 R	80000000	8.3145100E+00
2 RTLNP	20000000	+R*T*LN(1E-05*P)
3 V1	48000000	2.0368834E+04
4 V2	48000000	-2.9428630E+01
13 V11	48000000	-2.1733047E+04
14 V12	48000000	1.5210732E+01
17 V15	48000000	2.4203519E+04
18 V16	48000000	-8.3874195E+00
19 V17	48000000	3.0885837E+03
21 V19	48000000	2.2022284E+04
22 V20	48000000	-7.0401040E+00

LIQUID  
EXCESS MODEL IS REDLICH-KISTER\_MUGGIANU  
CONSTITUENTS: A,B

G(LIQUID,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +14000-10\*T  
G(LIQUID,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +18000-12\*T  
L(LIQUID,A,B;0) = 500.00<T< 2000.00: +V11+V12\*T  
L(LIQUID,A,B;1) = 500.00<T< 2000.00: +V13+V14\*T

A2B  
2 SUBLATTICES, SITES 2: 1  
CONSTITUENTS: A : B

G(A2B,A;B;0)- 2 G(BCC,A;0)-G(BCC,B;0) =  
500.00<T< 2000.00: +V1+V2\*T+V3\*T\*LN(T)

BCC  
EXCESS MODEL IS REDLICH-KISTER\_MUGGIANU  
CONSTITUENTS: A,B

G(BCC,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +0.0  
G(BCC,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +0.0  
L(BCC,A,B;0) = 500.00<T< 2000.00: +V15+V16\*T  
L(BCC,A,B;1) = 500.00<T< 2000.00: +V17+V18\*T

FCC  
EXCESS MODEL IS REDLICH-KISTER\_MUGGIANU  
CONSTITUENTS: A,B

G(FCC,A;0)-G(BCC,A;0) = 500.00<T< 2000.00: +408  
G(FCC,B;0)-G(BCC,B;0) = 500.00<T< 2000.00: +3300-3\*T  
L(FCC,A,B;0) = 500.00<T< 2000.00: +V19+V20\*T  
L(FCC,A,B;1) = 500.00<T< 2000.00: +V21+V22\*T

\$ ===== BLOCK NUMBER 1

DEFINED CONSTANTS  
DX=2E-2, P0=101325, DH=500, DT=10  
DEFINED FUNCTIONS AND VARIABLES%  
HTR=HM(LIQUID)-HM(A2B)

1 T=1193	1192.	10.0	-0.5777	-5.7769E-02
1 W(LIQUID,B)=0.408	0.4078	2.00E-02	-1.8752E-04	-9.3761E-03
1 W(BCC,B)=0.13	0.1303	2.00E-02	2.8316E-04	1.4158E-02
2 T=1341	1341.	10.0	0.2069	2.0690E-02
2 HTR=3727	3714.	5.00E+02	-12.84	-2.5688E-02
3 T=1049	1048.	10.0	-0.5117	-5.1171E-02
3 W(LIQUID,A)=0.27	0.2704	2.00E-02	3.8687E-04	1.9343E-02
3 W(BCC,A)=9.3E-2	9.3541E-02	2.00E-02	5.4112E-04	2.7056E-02
4 T=1203	1203.	10.0	0.1244	1.2439E-02
4 W(LIQUID,A)=0.19	0.1906	2.00E-02	5.5376E-04	2.7688E-02
4 W(BCC,A)=6.9E-2	6.9183E-02	2.00E-02	1.8326E-04	9.1632E-03
4 W(FCC,A)=6E-2	6.0276E-02	2.00E-02	2.7626E-04	1.3813E-02
5 T=726	725.5	10.0	-0.4879	-4.8791E-02
5 X(BCC,B)=3.7E-2	3.7429E-02	2.00E-02	4.2920E-04	2.1460E-02
5 X(BCC#2,A)=0.114	0.1141	2.00E-02	9.4014E-05	4.7007E-03
6 X(BCC,B)=3.7E-2	3.7567E-02	2.00E-02	5.6715E-04	2.8358E-02
6 X(BCC#2,A)=0.114	0.1144	2.00E-02	4.3136E-04	2.1568E-02
10 W(LIQUID,A)=2E-2	1.9551E-02	2.00E-02	-4.4908E-04	-2.2454E-02
11 W(LIQUID,A)=4.2E-2	4.1821E-02	2.00E-02	-1.7892E-04	-8.9460E-03
12 W(LIQUID,A)=6.5E-2	6.4884E-02	2.00E-02	-1.1630E-04	-5.8150E-03
13 W(LIQUID,A)=9.3E-2	9.2671E-02	2.00E-02	-3.2917E-04	-1.6458E-02
20 W(LIQUID,A)=0.104	0.1038	2.00E-02	-2.3309E-04	-1.1654E-02
20 W(FCC,A)=3.8E-2	3.8287E-02	2.00E-02	2.8690E-04	1.4345E-02
21 W(LIQUID,A)=0.136	0.1365	2.00E-02	4.7648E-04	2.3824E-02
21 W(FCC,A)=4.7E-2	4.7282E-02	2.00E-02	2.8217E-04	1.4109E-02

22	W(LIQUID,A)=0.187	0.1867	2.00E-02	-2.9105E-04	-1.4553E-02
22	W(FCC,A)=5.9E-2	5.9414E-02	2.00E-02	4.1416E-04	2.0708E-02
23	W(LIQUID,A)=0.245	0.2448	2.00E-02	-2.4851E-04	-1.2425E-02
23	W(BCC,A)=8.5E-2	8.5315E-02	2.00E-02	3.1454E-04	1.5727E-02
100	ACR(B)=0.94	0.9397	2.85E-02	-2.7275E-04	-9.5825E-03
101	ACR(B)=0.84	0.8395	2.82E-02	-4.7358E-04	-1.6802E-02
102	ACR(B)=0.74	0.7408	2.81E-02	7.7139E-04	2.7496E-02
103	ACR(B)=0.64	0.6424	2.81E-02	2.4449E-03	8.7112E-02
104	ACR(B)=0.54	0.5435	2.82E-02	3.5129E-03	0.1245
105	ACR(B)=0.44	0.4429	2.85E-02	2.9062E-03	0.1018
106	ACR(B)=0.34	0.3395	2.90E-02	-4.9853E-04	-1.7174E-02
107	ACR(B)=0.23	0.2321	2.97E-02	2.1003E-03	7.0704E-02
108	ACR(B)=0.12	0.1194	3.06E-02	-5.9355E-04	-1.9397E-02
110	HMR(LIQUID)=-1964	-1956.	5.00E+02	8.026	1.6052E-02
111	HMR(LIQUID)=-3500	-3477.	5.00E+02	22.71	4.5425E-02
112	HMR(LIQUID)=-4588	-4564.	5.00E+02	24.06	4.8120E-02
113	HMR(LIQUID)=-5239	-5216.	5.00E+02	23.07	4.6137E-02
114	HMR(LIQUID)=-5454	-5433.	5.00E+02	20.74	4.1476E-02
115	HMR(LIQUID)=-5233	-5216.	5.00E+02	17.07	3.4137E-02
116	HMR(LIQUID)=-4575	-4564.	5.00E+02	11.06	2.2120E-02
117	HMR(LIQUID)=-3481	-3477.	5.00E+02	3.712	7.4249E-03
118	HMR(LIQUID)=-1950	-1956.	5.00E+02	-5.974	-1.1948E-02

```

PARROT:
PARROT:
PARROT:Hit RETURN to continue
PARROT: @@ Calculate the phase diagram a final time.
PARROT: mac tcex36cpd
... the command in full is MACRO_FILE_OPEN
PARROT: set-echo
NO SUCH COMMAND, USE HELP
PARROT: @@ Calculate the phase diagram
PARROT: @@ This TCM should be run in PARROT
PARROT: go p-3
... the command in full is GOTO_MODULE
POLY_3:
POLY_3: @@ In PARROT, the global minimization is turned off automatically.
POLY_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning
POLY_3: @@ message will be given.
POLY_3:
POLY_3: advanced-option global yes,,
... the command in full is ADVANCED_OPTIONS
Settings for global minimization:
*** WARNING *** Global equilibrium calculation may create new composition sets
and this may corrupt your PARROT work file (.PAR file).
Do not go back to PARROT but exit from POLY after your POLY calculations.
POLY_3:
POLY_3: def-com,,,,
... the command in full is DEFINE_COMPONENTS
POLY_3: s-a-v 1 w(b) 0 1,,,,
... the command in full is SET_AXIS_VARIABLE
The condition W(B)=.1234 created
POLY_3: s-a-v 2 t 300 1700,,,,
... the command in full is SET_AXIS_VARIABLE
The condition T=942.2 created
POLY_3: s-c t=500
... the command in full is SET_CONDITION
POLY_3: l-c
... the command in full is LIST_CONDITIONS
W(B)=0.1234, P=1E5, N=1, T=500
DEGREES OF FREEDOM 0
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 412 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY_3: save tcex36 y
... the command in full is SAVE_WORKSPACES

```

This file contains results from a previous STEP or MAP command.  
The SAVE command will save the current status of the program but destroy  
the results from the previous STEP or MAP commands.

```

POLY_3: map
Version 5 mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

```

Organizing start points

Using ADDED start equilibria

```

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20

```

Working hard  
Generating start point 21  
Generating start point 22  
Generating start point 23  
Generating start point 24  
Generating start point 25  
Generating start point 26  
Generating start point 27  
Generating start point 28

Phase region boundary 1 at: 7.140E-01 3.100E+02  
BCC  
\*\* BCC#2  
Calculated.. 2 equilibria  
Terminating at axis limit.

Phase region boundary 2 at: 7.141E-01 3.000E+02  
BCC  
\*\* BCC#2  
Calculated. 14 equilibria

Phase region boundary 3 at: 6.819E-01 7.255E+02  
\*\* A2B  
BCC  
\*\* BCC#2

Phase region boundary 4 at: 3.626E-01 7.255E+02  
\*\* A2B  
BCC  
Calculated. 15 equilibria

Phase region boundary 5 at: 3.771E-01 1.192E+03  
\*\* LIQUID  
\*\* A2B  
BCC

Phase region boundary 6 at: 2.828E-01 1.192E+03  
\*\* LIQUID  
BCC  
Calculated 29 equilibria

Phase region boundary 7 at: 4.863E-01 1.192E+03  
\*\* LIQUID  
A2B  
Calculated. 28 equilibria

Phase region boundary 8 at: 6.500E-01 1.048E+03  
\*\* LIQUID  
A2B  
\*\* BCC

Phase region boundary 9 at: 7.639E-01 1.048E+03  
A2B  
\*\* BCC  
Calculated. 11 equilibria  
Terminating at known equilibrium

Phase region boundary 10 at: 8.272E-01 1.048E+03  
LIQUID  
\*\* BCC  
Calculated. 8 equilibria

Phase region boundary 11 at: 8.748E-01 1.203E+03  
LIQUID  
\*\* BCC  
\*\* FCC

Phase region boundary 12 at: 8.799E-01 1.203E+03  
LIQUID  
\*\* FCC  
Calculated 33 equilibria

Phase region boundary 13 at: 9.353E-01 1.203E+03  
BCC  
\*\* FCC  
Calculated 22 equilibria

Phase region boundary 14 at: 7.140E-01 3.100E+02  
BCC  
\*\* BCC#2  
Calculated. 13 equilibria  
Terminating at known equilibrium

Phase region boundary 15 at: 7.140E-01 3.100E+02  
BCC  
\*\* BCC#2  
Calculated.. 2 equilibria  
Terminating at known equilibrium  
Terminating at axis limit.

Phase region boundary 16 at: 7.140E-01 3.100E+02  
BCC  
\*\* BCC#2  
Calculated. 13 equilibria  
Terminating at known equilibrium

Phase region boundary 17 at: 7.140E-01 3.100E+02  
BCC  
\*\* BCC#2  
Calculated.. 2 equilibria  
Terminating at known equilibrium  
Terminating at axis limit.

Phase region boundary 18 at: 7.140E-01 3.100E+02  
BCC  
\*\* BCC#2  
Calculated. 13 equilibria  
Terminating at known equilibrium

Phase region boundary 19 at: 7.140E-01 3.100E+02  
BCC  
\*\* BCC#2  
Calculated.. 2 equilibria  
Terminating at known equilibrium  
Terminating at axis limit.

Phase region boundary 20 at: 7.140E-01 3.100E+02  
 BCC  
 \*\* BCC#2  
 Calculated. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 21 at: 7.140E-01 3.100E+02  
 \*\* BCC  
 BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 22 at: 7.140E-01 3.100E+02  
 \*\* BCC  
 BCC#2  
 Calculated. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 23 at: 7.140E-01 3.100E+02  
 \*\* BCC  
 BCC#2  
 Calculated.. 2 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 24 at: 7.140E-01 3.100E+02  
 \*\* BCC  
 BCC#2  
 Calculated. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 25 at: 3.647E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated 10 equilibria

Phase region boundary 26 at: 3.647E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated. 3 equilibria  
 Terminating at known equilibrium

Phase region boundary 27 at: 3.647E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated. 14 equilibria  
 Terminating at known equilibrium

Phase region boundary 28 at: 7.910E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated 10 equilibria

Phase region boundary 29 at: 7.910E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated. 3 equilibria  
 Terminating at known equilibrium

Phase region boundary 30 at: 7.910E-01 7.700E+02  
 \*\* A2B  
 BCC  
 Calculated. 9 equilibria  
 Terminating at known equilibrium

Phase region boundary 31 at: 2.448E-01 1.230E+03  
 \*\* LIQUID  
 BCC  
 Calculated. 4 equilibria  
 Terminating at known equilibrium

Phase region boundary 32 at: 2.448E-01 1.230E+03  
 \*\* LIQUID  
 BCC  
 Calculated 26 equilibria

Phase region boundary 33 at: 8.858E-01 1.230E+03  
 \*\* LIQUID  
 FCC  
 Calculated. 2 equilibria  
 Terminating at known equilibrium

Phase region boundary 34 at: 8.858E-01 1.230E+03  
 \*\* LIQUID  
 FCC  
 Calculated 29 equilibria

Phase region boundary 35 at: 6.415E-03 1.397E+03  
 LIQUID  
 \*\* BCC  
 Calculated 13 equilibria

Phase region boundary 36 at: 6.415E-03 1.397E+03  
 LIQUID  
 \*\* BCC  
 Calculated. 13 equilibria  
 Terminating at known equilibrium

Phase region boundary 37 at: 2.299E-01 1.244E+03  
 LIQUID  
 \*\* BCC  
 Calculated 20 equilibria

Phase region boundary 38 at: 2.299E-01 1.244E+03  
 LIQUID  
 \*\* BCC  
 Calculated. 4 equilibria  
 Terminating at known equilibrium

Phase region boundary 39 at: 6.122E-01 1.240E+03  
 LIQUID  
 \*\* A2B  
 Calculated. 14 equilibria  
 Terminating at known equilibrium



```

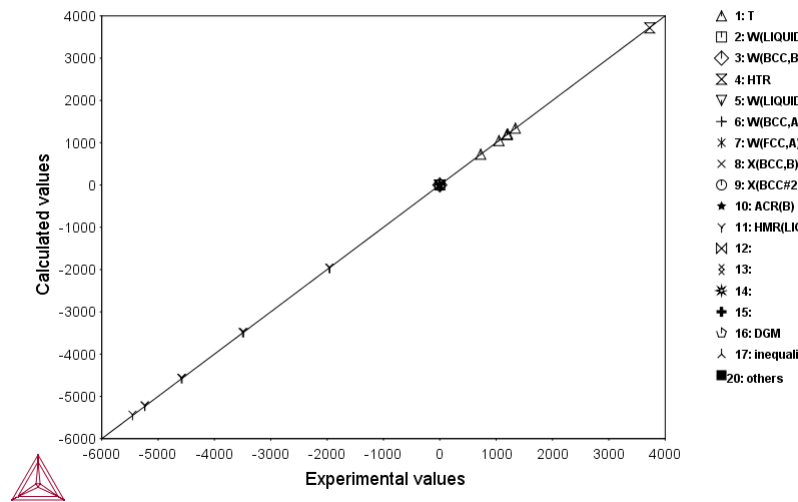
Phase region boundary 40 at: 6.122E-01 1.240E+03
LIQUID
** A2B
Calculated. 8 equilibria
Terminating at known equilibrium

Phase region boundary 41 at: 9.927E-01 1.613E+03
LIQUID
** FCC
Calculated. 20 equilibria
Terminating at known equilibrium

Phase region boundary 42 at: 9.927E-01 1.613E+03
LIQUID
** FCC
Calculated 13 equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tce
x36.POLY3
CPU time for mapping 1 seconds
POLY_3: post
POST: s-l d
... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
... the command in full is PLOT DIAGRAM
From PARROT optimization

2016.05.16.14.22.01
A,B
P=1E5,N=1

```



```

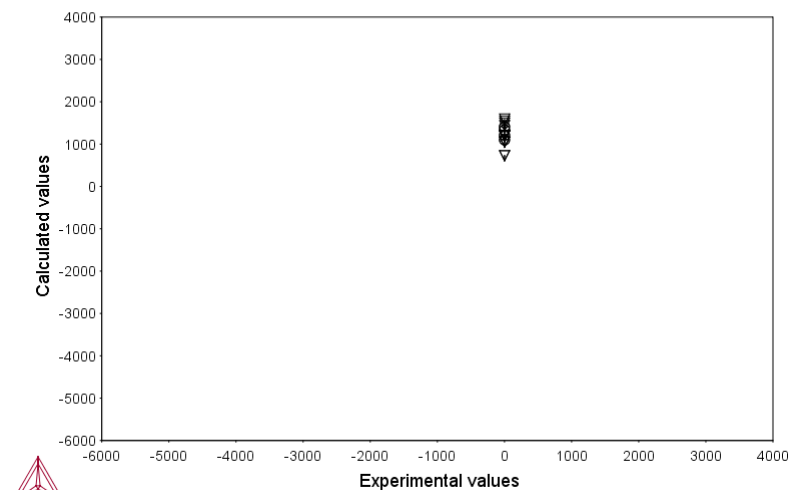
POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:Hit RETURN to continue
POST: @@ Add the experimental data
POST: a-e-d y exp36 0; 1
... the command in full is APPEND_EXPERIMENTAL_DATA
POST: plot
... the command in full is PLOT DIAGRAM
From PARROT optimization

```

```

2016.05.16.14.22.01
A,B
P=1E5,N=1

```



```

POST:
POST:
POST:Hit RETURN to continue
POST: @@ Also calculate the enthalpies in the liquid
POST: ba
... the command in full is BACK
POLY_3: read,,,
... the command in full is READ_WORKSPACES
POLY_3:
POLY_3:
POLY_3: s-a-v 2 none
... the command in full is SET_AXIS_VARIABLE
POLY_3: s-c t=1773
... the command in full is SET_CONDITION

```

```

POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated          412 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution          0 s, total time    0 s
POLY_3: sh hmr
... the command in full is SHOW_VALUE
HMR=13116.464
POLY_3: l-st c
... the command in full is LIST_STATUS
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS      REF. STATE      T(K)          P(Pa)
A              ENTERED    SER
B              ENTERED    SER
POLY_3: s-r-s a liq * 1e5
... the command in full is SET_REFERENCE_STATE
POLY_3: s-r-s b liq * 1e5
... the command in full is SET_REFERENCE_STATE
POLY_3: save tcex36h y
... the command in full is SAVE_WORKSPACES

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

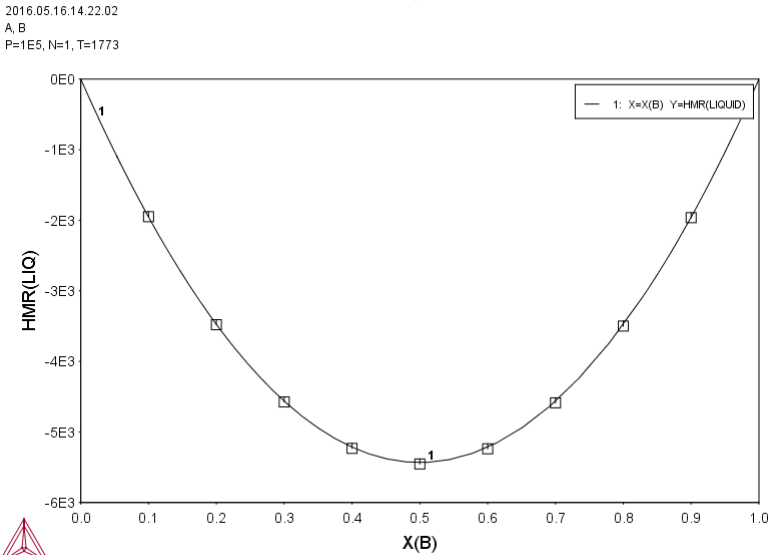
POLY_3: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value    0.123400
...OK

Phase Region from    0.123400    for:
LIQUID
Global test at    3.23400E-01 .... OK
Global test at    5.73400E-01 .... OK
Global test at    8.23400E-01 .... OK
Global test at    9.53400E-01 .... OK
Global test at    1.00000E+00 .... OK
Terminating at    1.00000
Calculated    51 equilibria

Phase Region from    0.123400    for:
LIQUID
Global test at    8.34000E-02 .... OK
Global test at    3.34000E-02 .... OK
Terminating at    0.25000E-11
Calculated    28 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tce
x36h.POLY3
POLY_3: post
POST: s-d-a x x(b)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y hmr(liq)
... the command in full is SET_DIAGRAM_AXIS
POST: a-e-d y exp36 0; 2
... the command in full is APPEND_EXPERIMENTAL_DATA
POST: plot
... the command in full is PLOT_DIAGRAM

```

From PARROT optimization



```

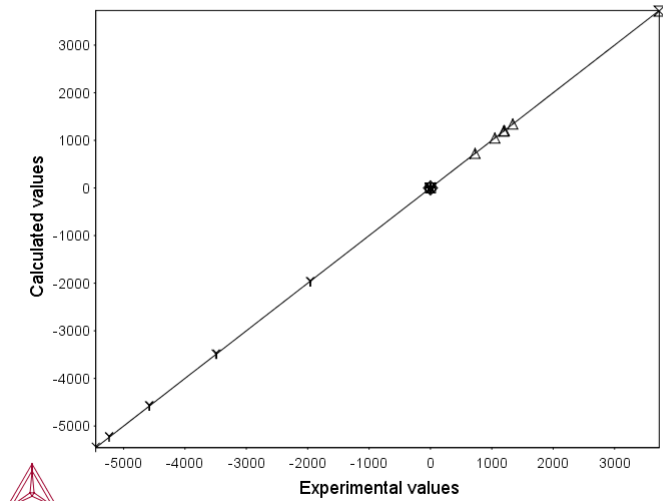
POST:
POST:Hit RETURN to continue
POST: @@ We can see the fitting results by the following method
POST: @@ Data points falling on the diagonal line indicates
POST: @@ perfect fitting.
POST: @@
POST: ba
... the command in full is BACK
POLY_3: ba
... the command in full is BACK

PARROT VERSION 5.3

Global minimization used as test only
PARROT: l-result gra pexp36 1,
... the command in full is LIST_RESULT
... the command in full is QUICK_EXPERIMENTAL_PLOT
... the command in full is PLOT_DIAGRAM

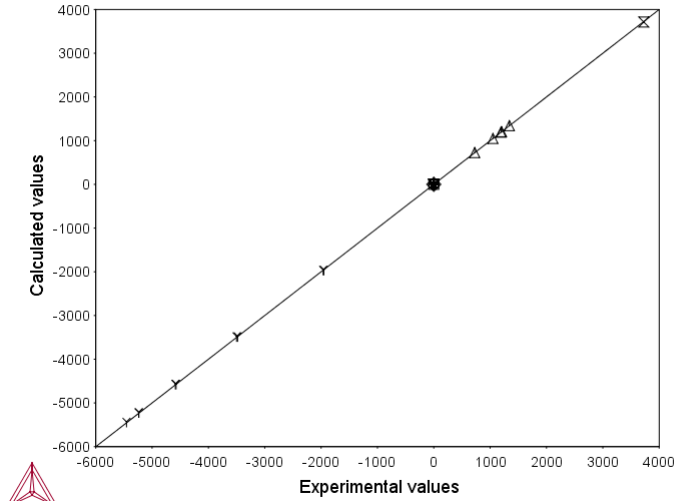
```

From PARROT optimization



POST: s-s-s y n -6000 4000  
... the command in full is SET\_SCALING\_STATUS  
POST: s-s-s x n -6000 4000  
... the command in full is SET\_SCALING\_STATUS  
POST: pl  
... the command in full is PLOT DIAGRAM

From PARROT optimization



POST: b  
... the command in full is BACK  
PARROT: set-inter  
... the command in full is SET\_INTERACTIVE  
PARROT:

## tcex36a-tcex36cpd

```
PARROT>AboutMACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tcex36cpd.TCM" set-echo
```

```
NO SUCH COMMAND, USE HELP
```

```
PARROT: @@ Calculate the phase diagram
```

```
PARROT: @@ This TCM should be run in PARROT
```

```
PARROT: go p-3
```

```
... the command in full is GOTO_MODULE
```

```
POLY_3:
```

```
POLY_3: @@ In PARROT, the global minimization is turned off automatically.
```

```
POLY_3: @@ Back in POLY-3, one needs to turn it on manually, but a warning
```

```
POLY_3: @@ message will be given.
```

```
POLY_3:
```

```
POLY_3: advanced-option global yes,,
```

```
... the command in full is ADVANCED_OPTIONS
```

```
Settings for global minimization:
```

```
*** WARNING *** Global equilibrium calculation may create new composition sets  
and this may corrupt your PARROT work file (.PAR file).
```

```
Do not go back to PARROT but exit from POLY after your POLY calculations.
```

```
POLY_3:
```

```
POLY_3: def-com,,,
```

```
... the command in full is DEFINE_COMPONENTS
```

```
POLY_3: s-a-v 1 w(b) 0 1,,,
```

```
... the command in full is SET_AXIS_VARIABLE
```

```
The condition W(B)=.1234 created
```

```
POLY_3: s-a-v 2 t 300 1700,,,
```

```
... the command in full is SET_AXIS_VARIABLE
```

```
The condition T=942.2 created
```

```
POLY_3: s-c t=500
```

```
... the command in full is SET_CONDITION
```

```
POLY_3: l-c
```

```
... the command in full is LIST_CONDITIONS
```

```
W(B)=0.1234, P=1E5, N=1, T=500
```

```
DEGREES OF FREEDOM 0
```

```
POLY_3: c-e
```

```
... the command in full is COMPUTE_EQUILIBRIUM
```

```
Using global minimization procedure
```

```
Calculated 412 grid points in 0 s
```

```
Found the set of lowest grid points in 0 s
```

```
Calculated POLY solution 0 s, total time 0 s
```

```
POLY_3: save tcex36 y
```

```
... the command in full is SAVE_WORKSPACES
```

```
This file contains results from a previous STEP or MAP command.
```

```
The SAVE command will save the current status of the program but destroy
```

```
the results from the previous STEP or MAP commands.
```

```
POLY_3: map
```

```
Version S mapping is selected
```

```
Generating start equilibrium 1
```

```
Generating start equilibrium 2
```

```
Generating start equilibrium 3
```

```
Generating start equilibrium 4
```

```
Generating start equilibrium 5
```

```
Generating start equilibrium 6
```

```
Generating start equilibrium 7
```

```
Generating start equilibrium 8
```

```
Generating start equilibrium 9
```

```
Generating start equilibrium 10
```

```
Generating start equilibrium 11
```

```
Generating start equilibrium 12
```

```
Organizing start points
```

```
Using ADDED start equilibria
```

```
Generating start point 1
```

```
Generating start point 2
```

```
Generating start point 3
```

```
Generating start point 4
```

```
Generating start point 5
```

```
Generating start point 6
```

```
Generating start point 7
```

```
Generating start point 8
```

```
Generating start point 9
```

```
Generating start point 10
```

```
Working hard
```

```
Generating start point 11
```

```
Generating start point 12
```

```
Generating start point 13
```

```
Generating start point 14
```

```
Generating start point 15
```

```
Generating start point 16
```

```
Generating start point 17
```

```
Generating start point 18
```

```
Generating start point 19
```

```
Generating start point 20
```

```
Working hard
```

```
Generating start point 21
```

```
Generating start point 22
```

```
Generating start point 23
```

```
Generating start point 24
```

```
Generating start point 25
```

```
Generating start point 26
```

```
Generating start point 27
```

```
Generating start point 28
```

```
Phase region boundary 1 at: 7.140E-01 3.100E+02
```

```
BCC
```

```
** BCC#2
```

```
Calculated.. 2 equilibria
```

```
Terminating at axis limit.
```

```
Phase region boundary 2 at: 7.141E-01 3.000E+02
```

```
BCC
```

```
** BCC#2
```

```
Calculated. 14 equilibria
```

```
Phase region boundary 3 at: 6.819E-01 7.255E+02
```

```
** A2B
```

```
BCC
```

```
** BCC#2
```

```
Phase region boundary 4 at: 3.626E-01 7.255E+02
```

```

** A2B
  BCC
Calculated.                15 equilibria

Phase region boundary  5 at:  3.771E-01  1.192E+03
** LIQUID
** A2B
  BCC

Phase region boundary  6 at:  2.828E-01  1.192E+03
** LIQUID
  BCC
Calculated                29 equilibria

Phase region boundary  7 at:  4.863E-01  1.192E+03
** LIQUID
  A2B
Calculated.              28 equilibria

Phase region boundary  8 at:  6.500E-01  1.048E+03
** LIQUID
  A2B
** BCC

Phase region boundary  9 at:  7.639E-01  1.048E+03
  A2B
** BCC
Calculated.              11 equilibria
Terminating at known equilibrium

Phase region boundary 10 at:  8.272E-01  1.048E+03
  LIQUID
** BCC
Calculated.              8 equilibria

Phase region boundary 11 at:  8.748E-01  1.203E+03
  LIQUID
** BCC
** FCC

Phase region boundary 12 at:  8.799E-01  1.203E+03
  LIQUID
** FCC
Calculated              33 equilibria

Phase region boundary 13 at:  9.353E-01  1.203E+03
  BCC
** FCC
Calculated              22 equilibria

Phase region boundary 14 at:  7.140E-01  3.100E+02
  BCC
** BCC#2
Calculated.             13 equilibria
Terminating at known equilibrium

Phase region boundary 15 at:  7.140E-01  3.100E+02
  BCC
** BCC#2
Calculated..             2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 16 at:  7.140E-01  3.100E+02
  BCC
** BCC#2
Calculated.             13 equilibria
Terminating at known equilibrium

Phase region boundary 17 at:  7.140E-01  3.100E+02
  BCC
** BCC#2
Calculated..             2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 18 at:  7.140E-01  3.100E+02
  BCC
** BCC#2
Calculated.             13 equilibria
Terminating at known equilibrium

Phase region boundary 19 at:  7.140E-01  3.100E+02
  BCC
** BCC#2
Calculated..             2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 20 at:  7.140E-01  3.100E+02
  BCC
** BCC#2
Calculated.             13 equilibria
Terminating at known equilibrium

Phase region boundary 21 at:  7.140E-01  3.100E+02
** BCC
  BCC#2
Calculated..             2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 22 at:  7.140E-01  3.100E+02
** BCC
  BCC#2
Calculated.             13 equilibria
Terminating at known equilibrium

Phase region boundary 23 at:  7.140E-01  3.100E+02
** BCC
  BCC#2
Calculated..             2 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 24 at:  7.140E-01  3.100E+02

```

```

** BCC
  BCC#2
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 25 at:  3.647E-01  7.700E+02
** A2B
  BCC
Calculated.          10 equilibria

Phase region boundary 26 at:  3.647E-01  7.700E+02
** A2B
  BCC
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 27 at:  3.647E-01  7.700E+02
** A2B
  BCC
Calculated.          14 equilibria
Terminating at known equilibrium

Phase region boundary 28 at:  7.910E-01  7.700E+02
** A2B
  BCC
Calculated.          10 equilibria

Phase region boundary 29 at:  7.910E-01  7.700E+02
** A2B
  BCC
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 30 at:  7.910E-01  7.700E+02
** A2B
  BCC
Calculated.          9 equilibria
Terminating at known equilibrium

Phase region boundary 31 at:  2.448E-01  1.230E+03
** LIQUID
  BCC
Calculated.          4 equilibria
Terminating at known equilibrium

Phase region boundary 32 at:  2.448E-01  1.230E+03
** LIQUID
  BCC
Calculated.          26 equilibria

Phase region boundary 33 at:  8.858E-01  1.230E+03
** LIQUID
  FCC
Calculated.          2 equilibria
Terminating at known equilibrium

Phase region boundary 34 at:  8.858E-01  1.230E+03
** LIQUID
  FCC
Calculated.          29 equilibria

Phase region boundary 35 at:  6.415E-03  1.397E+03
  LIQUID
** BCC
Calculated.          13 equilibria

Phase region boundary 36 at:  6.415E-03  1.397E+03
  LIQUID
** BCC
Calculated.          13 equilibria
Terminating at known equilibrium

Phase region boundary 37 at:  2.299E-01  1.244E+03
  LIQUID
** BCC
Calculated.          20 equilibria

Phase region boundary 38 at:  2.299E-01  1.244E+03
  LIQUID
** BCC
Calculated.          4 equilibria
Terminating at known equilibrium

Phase region boundary 39 at:  6.122E-01  1.240E+03
  LIQUID
** A2B
Calculated.          14 equilibria
Terminating at known equilibrium

Phase region boundary 40 at:  6.122E-01  1.240E+03
  LIQUID
** A2B
Calculated.          8 equilibria
Terminating at known equilibrium

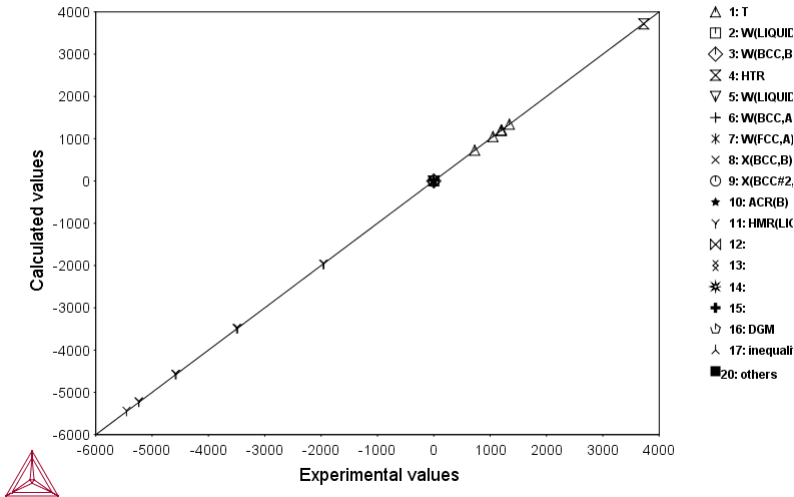
Phase region boundary 41 at:  9.927E-01  1.613E+03
  LIQUID
** FCC
Calculated.          20 equilibria
Terminating at known equilibrium

Phase region boundary 42 at:  9.927E-01  1.613E+03
  LIQUID
** FCC
Calculated.          13 equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex36a\tce
x36.POLY3
CPU time for mapping          1 seconds
POLY_3: post
POST: s-l d
... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
... the command in full is PLOT_DIAGRAM

```

From PARROT optimization

2016.05.16.14.23.00  
A, B  
P=1E5, N=1



POST:  
POST: set-inter  
... the command in full is SET\_INTERACTIVE\_MODE  
POST:

## tcex37

About Software (build 9533) running on WinNT 64-bit wordlength  
Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118  
License library version: 8.5.1.0017  
Linked: Mon May 16 09:31:44 2016

SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex37\tcex37.TCM" set-echo

SYS: @@

SYS: @@

SYS: @@ Calculation of an isothermal section, using command-lines

SYS: @@

SYS: set-log tcex37,,

SYS: go data

... the command in full is GOTO\_MODULE  
THERMODYNAMIC DATABASE module  
Current database: Steels/Fe-Alloys v8.0

VA DEFINED  
L12\_FCC B2\_BCC B2\_VACANCY  
HIGH\_SIGMA DICTRA\_FCC\_A1 REJECTED

TDB\_TCFE8: sw fedemo

... the command in full is SWITCH\_DATABASE  
Current database: Iron Demo Database

VA /- DEFINED

TDB\_FEDEMO: def-sys

... the command in full is DEFINE\_SYSTEM

ELEMENTS: fe cr ni

FE CR NI  
DEFINED

TDB\_FEDEMO: l-s c

... the command in full is LIST\_SYSTEM

LIQUID:L :CR FE NI:  
BCC\_A2 :CR FE NI:VA:  
CHI\_A12 :CR FE NI:CR:CR FE NI:  
FCC\_A1 :CR FE NI:VA:  
HCP\_A3 :CR FE NI:VA:  
LAVES\_PHASE\_C14 :CR FE NI:CR FE NI:  
SIGMA :CR FE NI:CR:CR FE NI:

TDB\_FEDEMO:Hit RETURN to continue

TDB\_FEDEMO: get

... the command in full is GET\_DATA

REINITIATING GES5 .....

ELEMENTS .....

SPECIES .....

PHASES .....

... the command in full is AMEND\_PHASE\_DESCRIPTION  
... the command in full is AMEND\_PHASE\_DESCRIPTION  
... the command in full is AMEND\_PHASE\_DESCRIPTION

PARAMETERS ...

FUNCTIONS ....

List of references for assessed data

'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'  
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'  
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Molar volumes'  
'X.-G. Lu et al. Calphad 29 (2005) 49-55, Fe P-T diagram'  
'J. Brillo and I. Egly, Int. J. Thermophysics, 24, pp. 1155-1170'  
'B.-J. Lee, Calphad (1993); revision of Fe-Cr and Fe-Ni liquid'  
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'J-O. Andersson and B. Sundman, Calphad, 11 (1987), 83-92; TRITA 0270  
(1986); CR-FE'  
'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR-NI'  
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'P. Gustafson, TRITA-MAC 342 (1987); CR-FE-W'  
'J-O. Andersson, Metall. Trans. A, 19A (1988), 1385-1394; TRITA 0322  
(1986); CR-FE-MO'  
'B.-J. Lee, estimated parameter 1999'  
'K. Frisk, Metall. Trans. A, 21A (1990), 2477-2488; TRITA 0409 (1989); CR  
-FE-N'  
'N. Saunders, COST 507 Report (1998); Cr-Ti'  
'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; LAVES\_PHASE\_C14'  
'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equil., 19 (1998),  
441-448; Fe-Ti'  
'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New  
Sigma model'  
'J. Bratberg, Thermo-Calc Software AB, Sweden, 2009; Fe-Cr-Ni'  
-OK-

TDB\_FEDEMO: go p-3

... the command in full is GOTO\_MODULE

POLY version 3.32

POLY\_3: l-st

... the command in full is LIST\_STATUS

Option /CPS/: cps

\*\*\* STATUS FOR ALL COMPONENTS

COMPONENT	STATUS	REF. STATE	T(K)	P(Pa)
VA	ENTERED	SER		
CR	ENTERED	SER		
FE	ENTERED	SER		
NI	ENTERED	SER		

\*\*\* STATUS FOR ALL PHASES

PHASE	STATUS	DRIVING FORCE	MOLES
SIGMA	ENTERED	0.000000E+00	0.000000E+00
LAVES_PHASE_C14	ENTERED	0.000000E+00	0.000000E+00
HCP_A3	ENTERED	0.000000E+00	0.000000E+00
FCC_A1	ENTERED	0.000000E+00	0.000000E+00
CHI_A12	ENTERED	0.000000E+00	0.000000E+00
BCC_A2	ENTERED	0.000000E+00	0.000000E+00
LIQUID	ENTERED	0.000000E+00	0.000000E+00

\*\*\* STATUS FOR ALL SPECIES

CR ENTERED FE ENTERED NI ENTERED VA ENTERED

POLY\_3: @@ Set conditions for a point inside the diagram

POLY\_3: s-c x(cr)=0.2 x(ni)=0.4

... the command in full is SET\_CONDITION

POLY\_3: s-c t=1673 p=1e5 n=1

... the command in full is SET\_CONDITION

POLY\_3: l-c

... the command in full is LIST\_CONDITIONS



```

X(CR)=0.2, X(NI)=0.4, T=1673, P=1E5, N=1
DEGREES OF FREEDOM 0
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      12633 grid points in      0 s
Found the set of lowest grid points in      0 s
Calculated POLY solution      0 s, total time      0 s
POLY_3: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
Output from POLY-3, equilibrium =      1, label A0 , database: FEDEMO

Conditions:
X(CR)=0.2, X(NI)=0.4, T=1673, P=1E5, N=1
DEGREES OF FREEDOM 0

Temperature  1673.00 K ( 1399.85 C), Pressure  1.000000E+05
Number of moles of components  1.00000E+00, Mass in grams  5.62140E+01
Total Gibbs energy -1.08423E+05, Enthalpy  4.89973E+04, Volume  7.34279E-06

Component      Moles      W-Fraction Activity Potential Ref.stat
CR              2.0000E-01  1.8499E-01  7.8623E-04 -9.9434E+04 SER
FE              4.0000E-01  3.9739E-01  4.0953E-04 -1.0851E+05 SER
NI              4.0000E-01  4.1762E-01  3.0004E-04 -1.1283E+05 SER

FCC_A1          Status ENTERED      Driving force  0.0000E+00
Moles 1.0000E+00, Mass 5.6214E+01, Volume fraction 1.0000E+00 Mass fractions:
NI  4.17618E-01 FE  3.97389E-01 CR  1.84993E-01
POLY_3: s-a-v
... the command in full is SET_AXIS_VARIABLE
Axis number: /1/: 1
Condition /NONE/: x(ni)
Min value /0/: 0
Max value /1/: 1
Increment /.025/: .025
POLY_3: s-a-v 2
... the command in full is SET_AXIS_VARIABLE
Condition /NONE/: x(cr)
Min value /0/: 0
Max value /1/: 1
Increment /.025/: .025
POLY_3: save tcex37 y
... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3: map
Version 3 mapping is selected
Generating start equilibrium  1
Generating start equilibrium  2
Generating start equilibrium  3
Generating start equilibrium  4
Generating start equilibrium  5
Generating start equilibrium  6
Generating start equilibrium  7
Generating start equilibrium  8
Generating start equilibrium  9

Organizing start points

Using ADDED start equilibria

Generating start point  1
Generating start point  2
Generating start point  3
Generating start point  4
Generating start point  5
Generating start point  6
Generating start point  7
Generating start point  8
Generating start point  9
Generating start point 10
Working hard
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16

Phase region boundary  1 at:   9.201E-03  4.019E-02
** BCC_A2
FCC_A1
Calculated      14 equilibria

Phase region boundary  2 at:   9.201E-03  4.019E-02
** BCC_A2
FCC_A1
Calculated.      31 equilibria

Phase region boundary  3 at:   1.950E-01  3.373E-01
** LIQUID
** BCC_A2
FCC_A1

Phase region boundary  4 at:   2.267E-01  3.103E-01
** LIQUID
FCC_A1
Calculated      53 equilibria

Phase region boundary  5 at:   1.883E-01  3.539E-01
** LIQUID
BCC_A2
Calculated      49 equilibria

Phase region boundary  6 at:   1.950E-01  3.373E-01
** BCC_A2
FCC_A1
Calculated      51 equilibria

Phase region boundary  7 at:   3.334E-01  3.082E-01
** LIQUID
FCC_A1
Calculated.      10 equilibria

```

```

Terminating at known equilibrium

Phase region boundary 8 at: 3.334E-01 3.082E-01
** LIQUID
FCC_A1
Calculated 39 equilibria

Phase region boundary 9 at: 6.543E-01 3.046E-01
** LIQUID
FCC_A1
Calculated. 35 equilibria
Terminating at known equilibrium

Phase region boundary 10 at: 6.543E-01 3.046E-01
** LIQUID
FCC_A1
Calculated 23 equilibria

Phase region boundary 11 at: 1.678E-01 3.000E-01
BCC_A2
** FCC_A1
Calculated 34 equilibria

Phase region boundary 12 at: 1.678E-01 3.000E-01
BCC_A2
** FCC_A1
Calculated. 4 equilibria
Terminating at known equilibrium

Phase region boundary 13 at: 3.086E-01 5.984E-01
** LIQUID
BCC_A2
Calculated. 21 equilibria
Terminating at known equilibrium

Phase region boundary 14 at: 3.086E-01 5.984E-01
** LIQUID
BCC_A2
Calculated 25 equilibria

Phase region boundary 15 at: 1.097E-02 4.525E-02
BCC_A2
** FCC_A1
Calculated 15 equilibria

Phase region boundary 16 at: 1.097E-02 4.525E-02
BCC_A2
** FCC_A1
Calculated. 31 equilibria
Terminating at known equilibrium

Phase region boundary 17 at: 3.342E-01 6.558E-01
LIQUID
** BCC_A2
Calculated. 26 equilibria
Terminating at known equilibrium

Phase region boundary 18 at: 3.342E-01 6.558E-01
LIQUID
** BCC_A2
Calculated 13 equilibria

Phase region boundary 19 at: 6.736E-01 3.160E-01
LIQUID
** FCC_A1
Calculated. 37 equilibria
Terminating at known equilibrium

Phase region boundary 20 at: 6.736E-01 3.160E-01
LIQUID
** FCC_A1
Calculated 18 equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex37\tcex
37.POLY3
CPU time for mapping 3 seconds
POLY_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

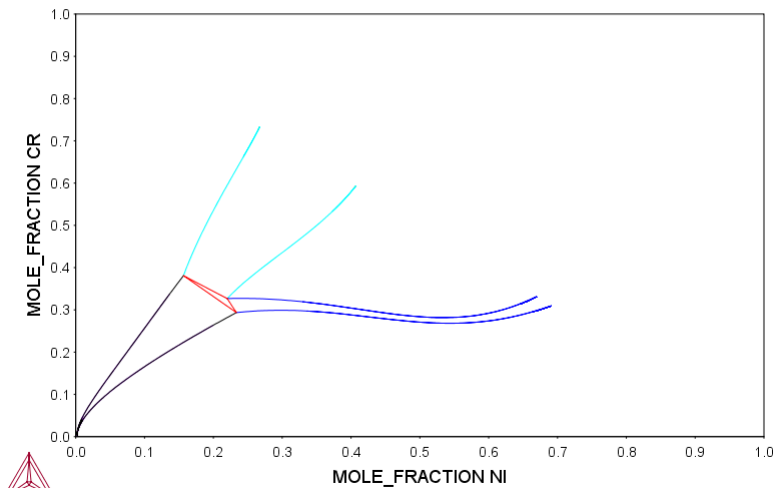
Setting automatic diagram axes

POST: @@ Use default axis on the diagram
POST:
POST: set-title example 37a
POST: plot
... the command in full is PLOT_DIAGRAM

```

### example 37a

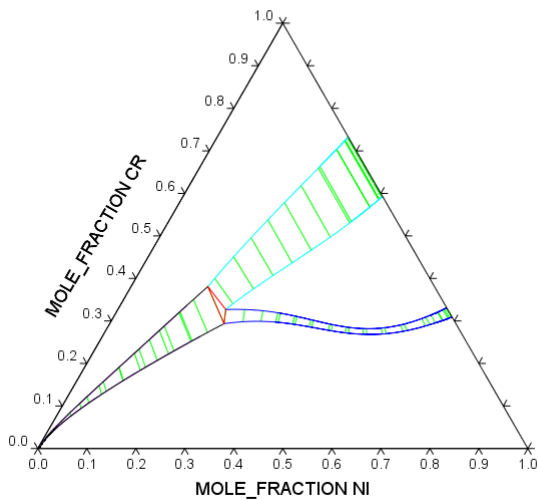
2016.05.16.14.25.10  
FEDEMO: CR, FE, NI  
T=1673, P=1E5, N=1



```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ By default a diagram is always square. set it triangular,
POST: @@ add tie-lines and set scaling on the axis
POST: s-d-t
... the command in full is SET_DIAGRAM_TYPE
TRIANGULAR DIAGRAM (Y OR N) /N/: y
POST: s-t-s
... the command in full is SET_TIELINE_STATUS
PLOTting EVERY TIE-LINE NO /0/: 3
POST: s-sc
... the command in full is SET_SCALING_STATUS
AXIS (X, Y OR Z) : x
AUTOMATIC SCALING (Y OR N) /N/: n
MIN VALUE : 0
MAX VALUE : 1
POST: s-s y n 0 1
... the command in full is SET_SCALING_STATUS
POST: set-title example 37b
POST:
POST: plot
... the command in full is PLOT DIAGRAM
```

### example 37b

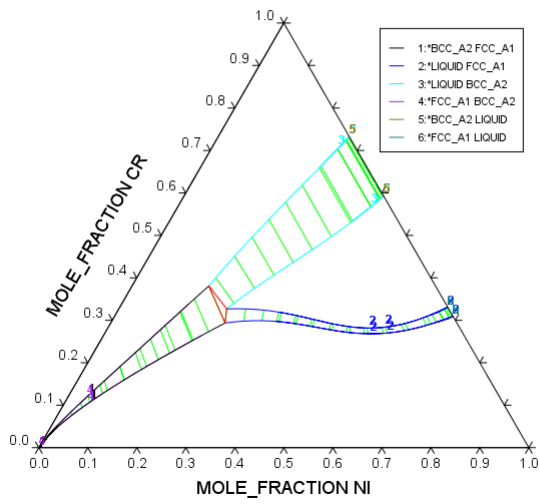
2016.05.16.14.25.10  
FEDEMO: CR, FE, NI  
T=1673, P=1E5, N=1



```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ To identify the phases also set labels
POST: @@ To add text in phase regions use a dataplot file
POST: set-lab b
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 37c
POST:
POST: plot
... the command in full is PLOT DIAGRAM
```

2016.05.16 14:25:11  
FEDEMO: CR, FE, NI  
T=1673, P=1E5, N=1

### example 37c



POST:  
POST: set-inter  
... the command in full is SET\_INTERACTIVE\_MODE  
POST:

tcex38

```
AboutMACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex38\tcex38.TCM" set-echo
SYS: @@
SYS: @@ Calculation of the Morral "rose"
SYS: @@
SYS: @@ Calculation of miscibility gaps ...
SYS: @@
SYS: set-log ex38,,,,
SYS: go g
... the command in full is GOTO_MODULE
GIBBS ENERGY SYSTEM version 5.2
GES: rei,,,,,
... the command in full is REINITIATE
GES:
GES: @@ Enter a phase with just a ternary interaction parameter
GES: e-e a b c
... the command in full is ENTER_ELEMENT
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
L12_FCC          B2_BCC          B2_VACANCY
HIGH_SIGMA      DICTRA_FCC_A1   REJECTED
GES: a-e-d a fcc_al 10,,,,,
... the command in full is AMEND_ELEMENT_DATA
GES: a-e-d b fcc_al 10,,,,,
... the command in full is AMEND_ELEMENT_DATA
GES: a-e-d c fcc_al 10,,,,,
... the command in full is AMEND_ELEMENT_DATA
GES:
GES:
GES: e-ph fcc_al,,1 A B C,,,,,
... the command in full is ENTER_PHASE
GES:
GES:
GES: e-par 1(fcc_al,a,b,c),,50000;,,,,
... the command in full is ENTER_PARAMETER
L(FCC_A1,A,B,C;0)
GES: l-d
... the command in full is LIST_DATA
OUTPUT TO SCREEN OR FILE /SCREEN/:
OPTIONS?:

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT          DATE 2016- 5-16
FROM DATABASE: User data 2016.05.16

ALL DATA IN SI UNITS
FUNCTIONS VALID FOR    298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

ELEMENT STABLE ELEMENT REFERENCE  MASS          H298-H0      S298
1 A   FCC_A1                      1.0000E+01   0.0000E+00   0.0000E+00
2 B   FCC_A1                      1.0000E+01   1.2220E+03   5.9000E+00
3 C   FCC_A1                      1.0000E+01   1.0540E+03   5.7400E+00

SPECIES                                STOICHIOMETRY
1 A                                    A
2 B                                    B
3 C                                    C

FCC_A1
EXCESS MODEL IS REDLICH-KISTER_MUGGIANU
CONSTITUENTS: A,B,C

G(FCC_A1,A;0)-G(FCC_A1,A;0) = 0.0
G(FCC_A1,B;0)-G(FCC_A1,B;0) = 0.0
G(FCC_A1,C;0)-G(FCC_A1,C;0) = 0.0
L(FCC_A1,A,B,C;0) = +50000

SYMBOL      STATUS  VALUE/FUNCTION
1 R          80000000  8.3145100E+00
2 RTLNP      20000000  +R*T*LN(1E-05*P)

GES: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3:
POLY_3: s-c t=600 p=1e5 n=1 x(b)=.3 x(c)=.1
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      1977 grid points in          0 s
Found the set of lowest grid points in        0 s
Creating a new composition set FCC_A1#2
Calculated POLY solution      0 s, total time    0 s
POLY_3: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/:
Output from POLY-3, equilibrium =      1, label A0 , database: User dat

Conditions:
T=600, P=1E5, N=1, X(B)=0.3, X(C)=0.1
DEGREES OF FREEDOM 0

Temperature      600.00 K ( 326.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 1.00000E+01
Total Gibbs energy -3.58989E+03, Enthalpy 6.74567E+02, Volume 0.00000E+00

Component      Moles      W-Fraction  Activity  Potential  Ref.stat
A                6.0000E-01   6.0000E-01  5.7356E-01 -2.7732E+03 SER
B                3.0000E-01   3.0000E-01  3.8092E-01 -4.8149E+03 SER
C                1.0000E-01   1.0000E-01  3.8092E-01 -4.8149E+03 SER

FCC_A1                      Status ENTERED      Driving force 0.0000E+00
Moles 8.7781E-01, Mass 8.7781E+00, Volume fraction 0.0000E+00 Mass fractions:
```

```

A 6.00000E-01 B 3.32342E-01 C 6.76579E-02

FCC_A1#2 Status ENTERED Driving force 0.0000E+00
Moles 1.2219E-01, Mass 1.2219E+00, Volume fraction 0.0000E+00 Mass fractions:
A 6.00000E-01 C 3.32342E-01 B 6.76579E-02
POLY_3:Hit RETURN to continue
POLY_3: s-a-v 1 x(b) 0 1 0.01
... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(c) 0 1 0.01
... the command in full is SET_AXIS_VARIABLE
POLY_3:
POLY_3: save tcex38 y
... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9

Organizing start points

Using ADDED start equilibria

Trying global minimization! 3
Generating start point 1
Generating start point 2
Trying global minimization! 3
Generating start point 3
Generating start point 4
Trying global minimization! 3
Generating start point 5
Generating start point 6
Trying global minimization! 3
Generating start point 7
Generating start point 8
Trying global minimization! 3
Generating start point 9
Generating start point 10
Working hard
Trying global minimization! 3
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14

Phase region boundary 1 at: 9.900E-01 1.000E-02
FCC_A1
** FCC_A1#2

+++++

Phase region boundary 2 at: 9.900E-01 1.000E-02
FCC_A1
** FCC_A1#2

+

Phase region boundary 3 at: 2.333E-01 2.333E-01
FCC_A1
** FCC_A1#2
Calculated 32 equilibria

Phase region boundary 4 at: 2.333E-01 2.333E-01
FCC_A1
** FCC_A1#2
Creating a new composition set FCC_A1#3
Calculated 11 equilibria

Phase region boundary 5 at: 2.333E-01 2.333E-01
FCC_A1
** FCC_A1#2
Calculated. 5 equilibria

Phase region boundary 6 at: 2.699E-01 2.699E-01
FCC_A1
** FCC_A1#2
** FCC_A1#3

Phase region boundary 7 at: 4.603E-01 2.699E-01
FCC_A1
** FCC_A1#3
Calculated 45 equilibria

Phase region boundary 8 at: 2.699E-01 4.603E-01
FCC_A1#2
** FCC_A1#3
Calculated 55 equilibria

Phase region boundary 9 at: 2.699E-01 2.699E-01
FCC_A1
** FCC_A1#2
Calculated 32 equilibria

Phase region boundary 10 at: 6.633E-01 1.683E-01
FCC_A1
** FCC_A1#2
Calculated 25 equilibria

Phase region boundary 11 at: 6.633E-01 1.683E-01
FCC_A1
** FCC_A1#2
Calculated 33 equilibria

Phase region boundary 12 at: 6.633E-01 1.683E-01
FCC_A1
** FCC_A1#2
Calculated. 22 equilibria
Terminating at known equilibrium

```

```

Phase region boundary 13 at: 2.333E-01 2.333E-01
  FCC_A1
  ** FCC_A1#2
Calculated 35 equilibria

Phase region boundary 14 at: 2.333E-01 2.333E-01
  FCC_A1
  ** FCC_A1#2
Calculated 11 equilibria

Phase region boundary 15 at: 2.333E-01 2.333E-01
  FCC_A1
  ** FCC_A1#2
Calculated. 5 equilibria
Terminating at known equilibrium

Phase region boundary 16 at: 1.683E-01 6.633E-01
  FCC_A1
  ** FCC_A1#2
Calculated 33 equilibria

Phase region boundary 17 at: 1.683E-01 6.633E-01
  FCC_A1
  ** FCC_A1#2
Calculated. 22 equilibria
Terminating at known equilibrium

Phase region boundary 18 at: 1.683E-01 6.633E-01
  FCC_A1
  ** FCC_A1#2
Calculated 28 equilibria

Phase region boundary 19 at: 2.333E-01 5.333E-01
  FCC_A1
  ** FCC_A1#2
Calculated 20 equilibria

Phase region boundary 20 at: 2.333E-01 5.333E-01
  FCC_A1
  ** FCC_A1#2
Calculated. 9 equilibria
Terminating at known equilibrium

Phase region boundary 21 at: 2.333E-01 5.333E-01
  FCC_A1
  ** FCC_A1#2
Calculated 44 equilibria

Phase region boundary 22 at: 6.633E-01 1.683E-01
  FCC_A1
  ** FCC_A1#2
Calculated 25 equilibria

Phase region boundary 23 at: 6.633E-01 1.683E-01
  FCC_A1
  ** FCC_A1#2
Calculated 33 equilibria

Phase region boundary 24 at: 6.633E-01 1.683E-01
  FCC_A1
  ** FCC_A1#2
Calculated. 22 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex38\tcex
38.POLY3
CPU time for mapping 2 seconds
POLY_3:
POLY_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

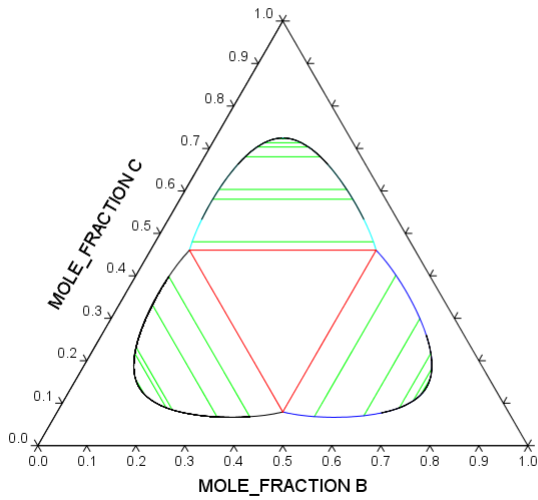
Setting automatic diagram axes

POST:
POST: s-d-a x m-f b
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y m-f c
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-ty y,,,,
... the command in full is SET_DIAGRAM_TYPE
POST: s-s x n 0 1
... the command in full is SET_SCALING_STATUS
POST: s-s y n 0 1
... the command in full is SET_SCALING_STATUS
POST: s-t-s 10
... the command in full is SET_TIELINE_STATUS
POST: set-title example 38a
POST: plot
... the command in full is PLOT_DIAGRAM
The composition set FCC_A1#3 created from the store file

```

# example 38a

2016.05.16 14:27:18  
User data 2016.05.16: A, B, C  
T=600, P=1E5, N=1



```
POST:
POST:Hit RETURN to continue
POST: back
POLY_3: read,,
... the command in full is READ_WORKSPACES
POLY_3:
POLY_3: @@ We will calculate at a higher temperature
POLY_3: @@ with a stable phase in the middle.
POLY_3: s-c t=696
... the command in full is SET_CONDITION
POLY_3: s-c x(b)=.44 x(c)=.28
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 1977 grid points in 0 s
Found the set of lowest grid points in 0 s
Creating a new composition set FCC_A1#3
Calculated POLY solution 0 s, total time 0 s
POLY_3:
POLY_3: save tcex38b y
... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9

Organizing start points

Using ADDED start equilibria

Working hard
Trying global minimization! 3
Generating start point 1
Generating start point 2
Trying global minimization! 3
Generating start point 3
Generating start point 4
Trying global minimization! 3
Generating start point 5
Generating start point 6

Phase region boundary 1 at: 2.683E-01 2.683E-01
FCC_A1
** FCC_A1#2
Calculated 33 equilibria

Phase region boundary 2 at: 2.683E-01 2.683E-01
FCC_A1
** FCC_A1#2
Calculated 6 equilibria

Phase region boundary 3 at: 2.683E-01 2.683E-01
FCC_A1
** FCC_A1#2
Calculated 6 equilibria

Phase region boundary 4 at: 2.683E-01 2.683E-01
FCC_A1
** FCC_A1#2
Calculated 6 equilibria

Phase region boundary 5 at: 2.683E-01 2.683E-01
FCC_A1
** FCC_A1#2
Calculated 6 equilibria

Phase region boundary 6 at: 2.683E-01 2.683E-01
FCC_A1
** FCC_A1#2
Calculated 6 equilibria

Phase region boundary 7 at: 2.683E-01 2.683E-01
```



```

    FCC_A1
** FCC_A1#2
Calculated.                6 equilibria

Phase region boundary  8 at:  2.998E-01  2.998E-01
    FCC_A1
** FCC_A1#2
** FCC_A1#3

Phase region boundary  9 at:  3.618E-01  2.650E-01
    FCC_A1
** FCC_A1#3
Calculated                8 equilibria

Phase region boundary 10 at:  3.618E-01  2.650E-01
    FCC_A1
** FCC_A1#3
Calculated.                6 equilibria

Phase region boundary 11 at:  3.732E-01  2.650E-01
    FCC_A1
** FCC_A1#2
** FCC_A1#3

Phase region boundary 12 at:  4.004E-01  2.998E-01
    FCC_A1
** FCC_A1#2
Calculated                34 equilibria

Phase region boundary 13 at:  3.732E-01  3.618E-01
** FCC_A1#2
    FCC_A1#3
Calculated                4 equilibria

Phase region boundary 14 at:  3.732E-01  3.618E-01
** FCC_A1#2
    FCC_A1#3
Calculated.                3 equilibria

Phase region boundary 15 at:  3.618E-01  3.732E-01
** FCC_A1
** FCC_A1#2
    FCC_A1#3

Phase region boundary 16 at:  2.650E-01  3.732E-01
** FCC_A1
    FCC_A1#3
Calculated                9 equilibria

Phase region boundary 17 at:  2.650E-01  3.732E-01
** FCC_A1
    FCC_A1#3
Calculated.                7 equilibria
Terminating at known equilibrium

Phase region boundary 18 at:  2.998E-01  4.004E-01
** FCC_A1
    FCC_A1#2
Calculated                37 equilibria

Phase region boundary 19 at:  2.998E-01  2.998E-01
    FCC_A1
** FCC_A1#2
Calculated                40 equilibria

Phase region boundary 20 at:  2.683E-01  2.683E-01
    FCC_A1
** FCC_A1#2
Calculated                35 equilibria

Phase region boundary 21 at:  2.683E-01  2.683E-01
    FCC_A1
** FCC_A1#2
Calculated                6 equilibria

Phase region boundary 22 at:  2.683E-01  2.683E-01
    FCC_A1
** FCC_A1#2
Calculated                6 equilibria

Phase region boundary 23 at:  2.683E-01  2.683E-01
    FCC_A1
** FCC_A1#2
Calculated                6 equilibria

Phase region boundary 24 at:  2.683E-01  2.683E-01
    FCC_A1
** FCC_A1#2
Calculated                6 equilibria

Phase region boundary 25 at:  2.683E-01  2.683E-01
    FCC_A1
** FCC_A1#2
Calculated                6 equilibria

Phase region boundary 26 at:  2.683E-01  2.683E-01
    FCC_A1
** FCC_A1#2
Calculated.                6 equilibria
Terminating at known equilibrium

Phase region boundary 27 at:  2.683E-01  4.633E-01
    FCC_A1
** FCC_A1#2
Calculated.                9 equilibria
Creating a new composition set FCC_A1#4
Calculated                9 equilibria

Phase region boundary 28 at:  2.683E-01  4.633E-01
    FCC_A1
** FCC_A1#2
Calculated                9 equilibria

Phase region boundary 29 at:  2.683E-01  4.633E-01
    FCC_A1
** FCC_A1#2

```

```

Calculated                      9 equilibria

Phase region boundary 30 at:    2.683E-01  4.633E-01
  FCC_A1
  ** FCC_A1#2
Calculated                      9 equilibria

Phase region boundary 31 at:    2.683E-01  4.633E-01
  FCC_A1
  ** FCC_A1#2
Calculated                      9 equilibria

Phase region boundary 32 at:    2.683E-01  4.633E-01
  FCC_A1
  ** FCC_A1#2
Calculated.                    9 equilibria
Terminating at known equilibrium

Phase region boundary 33 at:    2.683E-01  4.633E-01
  FCC_A1
  ** FCC_A1#2
Calculated                    31 equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex38\tcex
38b.POLY3
CPU time for mapping              3 seconds
POLY_3:
POLY_3:
POLY_3: post

```

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

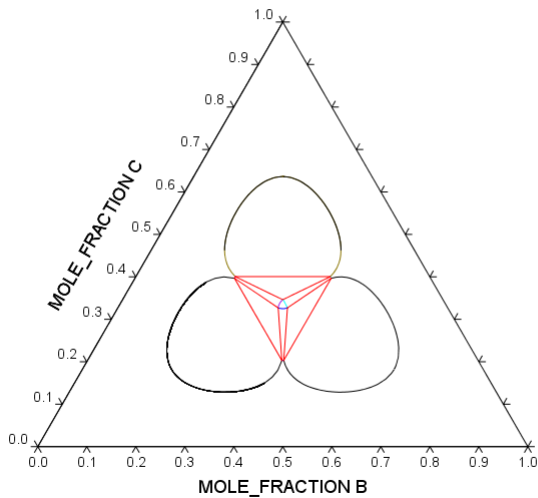
```

POST:
POST:
POST: set-title example 38b
POST: s-d-ty y,,,,
... the command in full is SET_DIAGRAM_TYPE
POST: s-s x n 0 1
... the command in full is SET_SCALING_STATUS
POST: s-s y n 0 1
... the command in full is SET_SCALING_STATUS
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
The composition set FCC A1#4 created from the store file

```

**example 38b**

2016.05.16.14.27.22  
 User data 2016.05.16: A, B, C  
 T=696, P=1E5, N=1



```

POST:
POST:Hit RETURN to continue
POST:
POST: back
POLY_3: @@ =====
POLY_3: @@ Now a quaternary!
POLY_3: @@
POLY_3: @@ Square rose by John Morral
POLY_3: @@
POLY_3: go g
... the command in full is GOTO_MODULE
GIBBS ENERGY SYSTEM version 5.2
GES: rei,,,,
... the command in full is REINITIATE
GES: e-e a b c d
... the command in full is ENTER_ELEMENT
GES: a-e-d a liquid 10,,,,
... the command in full is AMEND_ELEMENT_DATA
GES: a-e-d b liquid 10,,,,
... the command in full is AMEND_ELEMENT_DATA
GES: a-e-d c liquid 10,,,,
... the command in full is AMEND_ELEMENT_DATA
GES: a-e-d d liquid 10,,,,
... the command in full is AMEND_ELEMENT_DATA
GES: e-ph liquid
... the command in full is ENTER_PHASE
TYPE CODE:
NUMBER OF SUBLATTICES /1/: 1
NAME OF CONSTITUENT: A B C D
NAME OF CONSTITUENT:
WILL YOU ADD CONSTITUENTS LATER /NO/: NO
DO YOU WANT A LIST OF POSSIBLE PARAMETERS /NO/: NO
GES: e-par g(liquid,a,b,c,d)

```

```

... the command in full is ENTER_PARAMETER
G(LIQUID,A,B,C,D;0)
LOW TEMPERATURE LIMIT /298.15/: 298.15
FUNCTION: 100000
6
HIGH TEMPERATURE LIMIT /6000/: 6000
ANY MORE RANGES /N/: N
GES:
GES: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3: rei,,,,
... the command in full is REINITIATE_MODULE
POLY_3: s-c t=170 p=1e5 n=1 x(d)=.25 x(a)=.3 x(a)+x(c)=.5
... the command in full is SET_CONDITION
POLY_3: l-c
... the command in full is LIST_CONDITIONS
T=170, P=1E5, N=1, X(D)=0.25, X(A)=0.3, X(A)+X(C)=0.5
DEGREES OF FREEDOM 0
POLY_3:
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 1819 grid points in 0 s
Creating a new composition set LIQUID#2
32 ITS, CPU TIME USED 0 SECONDS
POLY_3: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VXCS
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=170, P=1E5, N=1, X(D)=0.25, X(A)=0.3, X(A)+X(C)=0.5
DEGREES OF FREEDOM 0

Temperature 170.00 K ( -103.15 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 1.00000E+01
Total Gibbs energy -1.58399E+03, Enthalpy 2.18612E+02, Volume 0.00000E+00

Component      Moles      M-Fraction  Activity   Potential  Ref.stat
A                3.0000E-01  3.0000E-01  3.1587E-01 -1.6289E+03 SER
B                2.5000E-01  2.5000E-01  3.5423E-01 -1.4669E+03 SER
C                2.0000E-01  2.0000E-01  3.5423E-01 -1.4669E+03 SER
D                2.5000E-01  2.5000E-01  2.9182E-01 -1.7409E+03 SER

LIQUID          Status ENTERED   Driving force 0.0000E+00
Moles 5.8530E-01, Mass 5.8530E+00, Volume fraction 0.0000E+00 Mole fractions:
B 3.71549E-01 A 3.00000E-01 D 2.50000E-01 C 7.84507E-02

LIQUID#2        Status ENTERED   Driving force 0.0000E+00
Moles 4.1470E-01, Mass 4.1470E+00, Volume fraction 0.0000E+00 Mole fractions:
C 3.71549E-01 A 3.00000E-01 D 2.50000E-01 B 7.84507E-02
POLY_3: s-a-v 1 x(a)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: .5
Increment /.0125/: .01
POLY_3: s-a-v 2 x(d)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: 0
Max value /1/: .5
Increment /.0125/: .01
POLY_3:
POLY_3: add +1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: save tcex38c y
... the command in full is SAVE_WORKSPACES
POLY_3: map
Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Tie-lines not in the plane of calculation
Generating start point 1
Generating start point 2

Phase region boundary 1 at: 4.478E-01 2.500E-01
LIQUID
** LIQUID#2
Creating a new composition set LIQUID#3
Calculated 6 equilibria

Phase region boundary 2 at: 4.478E-01 2.500E-01
LIQUID
** LIQUID#2
Calculated 2 equilibria

Phase region boundary 3 at: 4.478E-01 2.500E-01
LIQUID
** LIQUID#2
Calculated 2 equilibria

Phase region boundary 4 at: 4.478E-01 2.500E-01
LIQUID
** LIQUID#2
Calculated 2 equilibria

Phase region boundary 5 at: 4.478E-01 2.500E-01
LIQUID
** LIQUID#2
Calculated 2 equilibria

Phase region boundary 6 at: 4.478E-01 2.500E-01
LIQUID
** LIQUID#2
Calculated 2 equilibria
Calculated 2 equilibria

```

```

Phase region boundary 7 at: 4.478E-01 2.500E-01
LIQUID
** LIQUID#2
Calculated 45 equilibria

Phase region boundary 8 at: 4.478E-01 2.500E-01
LIQUID
** LIQUID#2
Calculated. 41 equilibria

Phase region boundary 9 at: 2.500E-01 4.478E-01
LIQUID
** LIQUID#2
** LIQUID#3

Phase region boundary 10 at: 2.500E-01 4.478E-01
LIQUID
** LIQUID#2
LIQUID#3
Creating a new composition set LIQUID#4
Calculated 31 equilibria

Phase region boundary 11 at: 2.500E-01 4.478E-01
LIQUID
** LIQUID#2
LIQUID#3
Calculated. 15 equilibria

Phase region boundary 12 at: 1.816E-01 3.184E-01
LIQUID
** LIQUID#2
LIQUID#3
** LIQUID#4

Phase region boundary 13 at: 3.184E-01 3.184E-01
LIQUID
LIQUID#2
** LIQUID#3
Calculated. 15 equilibria
Terminating at known equilibrium

Phase region boundary 14 at: 3.184E-01 3.184E-01
LIQUID
LIQUID#2
** LIQUID#4
Calculated. 14 equilibria

Phase region boundary 15 at: 4.478E-01 2.500E-01
** LIQUID
LIQUID#2
** LIQUID#4

Phase region boundary 16 at: 4.478E-01 2.500E-01
LIQUID#2
** LIQUID#4
Calculated. 43 equilibria

Phase region boundary 17 at: 2.500E-01 5.217E-02
LIQUID#2
** LIQUID#3
** LIQUID#4

Phase region boundary 18 at: 2.500E-01 5.217E-02
LIQUID#2
LIQUID#3
** LIQUID#4
Calculated 20 equilibria

Phase region boundary 19 at: 2.500E-01 5.217E-02
LIQUID#2
LIQUID#3
** LIQUID#4
Calculated. 15 equilibria
Terminating at known equilibrium

Phase region boundary 20 at: 2.500E-01 5.217E-02
LIQUID#2
** LIQUID#3
Calculated. 41 equilibria

Phase region boundary 21 at: 5.217E-02 2.500E-01
LIQUID#2
** LIQUID#3
** LIQUID#4

Phase region boundary 22 at: 5.217E-02 2.500E-01
LIQUID#2
** LIQUID#3
LIQUID#4
Calculated 20 equilibria

Phase region boundary 23 at: 5.217E-02 2.500E-01
LIQUID#2
** LIQUID#3
LIQUID#4
Calculated. 15 equilibria
Terminating at known equilibrium

Phase region boundary 24 at: 5.217E-02 2.500E-01
LIQUID#2
** LIQUID#4
Calculated. 41 equilibria
Terminating at known equilibrium

Phase region boundary 25 at: 5.217E-02 2.500E-01
LIQUID#2
LIQUID#3
** LIQUID#4
Calculated. 15 equilibria
Terminating at known equilibrium

Phase region boundary 26 at: 2.500E-01 5.217E-02
LIQUID#2
** LIQUID#3
LIQUID#4
Calculated 20 equilibria

```

Phase region boundary 27 at: 2.500E-01 5.217E-02  
LIQUID#2  
\*\* LIQUID#3  
LIQUID#4  
Calculated. 15 equilibria  
Terminating at known equilibrium

Phase region boundary 28 at: 4.478E-01 2.500E-01  
\*\* LIQUID  
LIQUID#2  
Calculated. 43 equilibria  
Terminating at known equilibrium

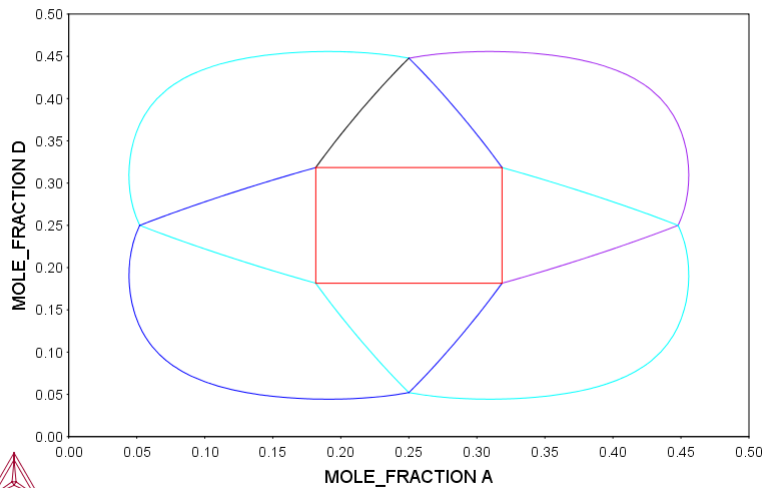
Phase region boundary 29 at: 4.478E-01 2.500E-01  
\*\* LIQUID  
LIQUID#2  
LIQUID#4  
Calculated. 15 equilibria  
Terminating at known equilibrium  
\*\*\* BUFFER SAVED ON FILE:  
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex38\tcex38c.POLY3  
CPU time for mapping 1 seconds  
**POLY\_3:** post

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

**POST:**  
**POST:**  
**POST:** set-title example 38c  
**POST:**  
**POST:** plot  
... the command in full is PLOT\_DIAGRAM  
The composition set LIQUID#3 created from the store file  
**example 38c**

2016.05.16.14.27.26  
User data 2016.05.16: A, B, C, D  
T=170, P=1E5, N=1, X(A)+X(C)=0.5



**POST:**  
**POST:** set-inter  
... the command in full is SET\_INTERACTIVE\_MODE  
**POST:**

```

AboutMACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex39.TCM" set-echo
SYS: @@
SYS: @@
SYS: @@ The Calculation of the Reversible Carnot Cycle of Heat Engine
SYS: @@
SYS: @@
SYS: @@ The Reversible Carnot cycles are usually drawn schematically in lectures
SYS: @@ or text books and rarely understood by students. But by making use of
SYS: @@ a thermodynamic software system like Thermo-Calc and realistic data it
SYS: @@ is possible to calculate a reversible Carnot cycle of a heat engine
SYS: @@ and to relate it to different thermodynamic quantities.
SYS: @@ Some particular cases will be calculated and graphically presented in this
SYS: @@ example.
SYS: @@
SYS: @@
SYS: @@ One application of the Second Law is to the efficiencies of heat
SYS: @@ engines, pumps and refrigerators.
SYS: @@ Whenever there exists a difference of temperature, work can be
SYS: @@ produced - the principle of heat engines. The Gibbs energy also
SYS: @@ enables us to predict the maximum work that a process may achieve.
SYS: @@
SYS: @@
SYS: @@ To illustrate how Thermo-Calc calculates the reversible Carnot cycle we
SYS: @@ will consider one mole of an ideal gas with two fictitious species A
SYS: @@ and A2.
SYS: set-log ex39,,,
SYS:
SYS: go g
... the command in full is GOTO_MODULE
GIBBS ENERGY SYSTEM version 5.2
GES: rei,,,,
... the command in full is REINITIATE
GES: e-e a
... the command in full is ENTER_ELEMENT
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
L12_FCC B2_BCC B2_VACANCY
HIGH_SIGMA DICTRA_FCC_A1 REJECTED
GES: a-e-d a gas 10,,,
... the command in full is AMEND_ELEMENT_DATA
GES: e-sp A2 A2
... the command in full is ENTER_SPECIES
GES: e-ph gas g 1 A A2; N N
... the command in full is ENTER_PHASE
GES: @@ The Gibbs free energy for these specie could be described by
GES: @@ the general formula:  $G_m = a + bT + c \ln T + dT^2 + \dots + RT \ln(P)$ 
GES: @@
GES: @@ In order to calculate the Carnot cycle one has to give some numerical
GES: @@ values to the a, b, c, etc. constants of the Gm expression.
GES: @@ It is important to understand that the coefficients cannot be
GES: @@ chosen arbitrarily, for example c should be negative as the heat capacity
GES: @@ at constant pressure,  $C_p = -T d^2G/dT^2$  and thus  $C_p = -c - 2dT$  must always be  $>0$ 
GES: @@
GES: e-par g(gas,a) 298.15 6960-51*T-17*T*LN(T)+R*T*LN(1e-05*P);,,,
... the command in full is ENTER_PARAMETER
G(GAS,A;0)-G(GAS,A;0)
GES: e-par g(gas,a2) 298.15 130670-38*T-17*T*LN(T)+R*T*LN(1e-05*P);,,,
... the command in full is ENTER_PARAMETER
G(GAS,A2;0)-2 G(GAS,A;0)
GES: l-d,,,
... the command in full is LIST_DATA

1OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT DATE 2016- 5-16
FROM DATABASE: User data 2016.05.16

ALL DATA IN SI UNITS
FUNCTIONS VALID FOR 298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

ELEMENT STABLE ELEMENT REFERENCE MASS H298-H0 S298
1 A GAS 1.0000E+01 0.0000E+00 0.0000E+00

SPECIES STOICHIOMETRY
1 A A
2 A2 A2

GAS
CONSTITUENTS: A,A2

G(GAS,A;0)-G(GAS,A;0) = +6960-51*T-17*T*LN(T)+R*T*LN(1E-05*P)
G(GAS,A2;0)-2 G(GAS,A;0) = +130670-38*T-17*T*LN(T)+R*T*LN(1E-05*P)

SYMBOL STATUS VALUE/FUNCTION
1 R 80000000 8.3145100E+00
2 RTLNP 20000000 +R*T*LN(1E-05*P)

GES:Hit RETURN to continue
GES: @@
GES: @@ The Carnot cycle diagram gives the pressure and volume for the
GES: @@ working media of a heat engine that operates between two temperatures
GES: @@ T1 and T2, T1>T2.
GES: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3: @@ The Carnot cycle will be calculated for T1=500 K (the temperature
POLY_3: @@ of the hot reservoir) and T2=400 K (the temperature of the cold
POLY_3: @@ reservoir)
POLY_3: ent var t1=500;
... the command in full is ENTER_SYMBOL
POLY_3: ent var t2=400;
... the command in full is ENTER_SYMBOL
POLY_3: @@

```

```

POLY_3: @@ A Carnot cycle consists of four reversible stages:
POLY_3: @@
POLY_3: @@ Stage 1. Isothermal expansion at T1; the entropy change of the system is
POLY_3: @@ Q1/T1, where Q1 is the heat taken from the hot reservoir.
POLY_3: @@
POLY_3: @@
POLY_3: s-c t=t1 p=1e7 n=1
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 137 grid points in 0 s
POLY_3: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: xn
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=T1, P=1E7, N=1
DEGREES OF FREEDOM 0

Temperature 500.00 K ( 226.85 C), Pressure 1.000000E+07
Number of moles of components 1.00000E+00, Mass in grams 1.00000E+01
Total Gibbs energy -5.22193E+04, Enthalpy 1.54600E+04, Volume 4.15725E-04

Component      Moles      M-Fraction Activity Potential Ref.stat
A               1.0000E+00  1.0000E+00 3.5061E-06 -5.2219E+04 SER

GAS              Status ENTERED Driving force 0.0000E+00
Moles 1.0000E+00, Mass 1.0000E+01, Volume fraction 1.0000E+00 Mole fractions:
A 1.00000E+00
Constitution:
A 1.00000E+00 A2 8.75433E-20
POLY_3:Hit RETURN to continue
POLY_3: @@ Set volume to 1 m3
POLY_3: s-c v
... the command in full is SET_CONDITION
Value /4.15725E-04/: 1
POLY_3: s-c n
... the command in full is SET_CONDITION
Value /1/: none
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Using already calculated grid
6 ITS, CPU TIME USED 0 SECONDS
POLY_3: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=T1, P=1E7, V=1
DEGREES OF FREEDOM 0

Temperature 500.00 K ( 226.85 C), Pressure 1.000000E+07
Number of moles of components 2.40543E+03, Mass in grams 2.40543E+04
Total Gibbs energy -1.25610E+08, Enthalpy 3.71880E+07, Volume 1.00000E+00

Component      Moles      M-Fraction Activity Potential Ref.stat
A               2.4054E+03  1.0000E+00 3.5061E-06 -5.2219E+04 SER

GAS              Status ENTERED Driving force 0.0000E+00
Moles 2.4054E+03, Mass 2.4054E+04, Volume fraction 1.0000E+00 Mole fractions:
A 1.00000E+00
Constitution:
A 1.00000E+00 A2 8.75433E-20
POLY_3: s-c n
... the command in full is SET_CONDITION
Value /2405.433393/:
POLY_3: s-c p
... the command in full is SET_CONDITION
Value /10000000/: none
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Using already calculated grid
6 ITS, CPU TIME USED 0 SECONDS
POLY_3: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=T1, N=2405.43, V=1
DEGREES OF FREEDOM 0

Temperature 500.00 K ( 226.85 C), Pressure 1.000000E+07
Number of moles of components 2.40543E+03, Mass in grams 2.40543E+04
Total Gibbs energy -1.25610E+08, Enthalpy 3.71880E+07, Volume 1.00000E+00

Component      Moles      M-Fraction Activity Potential Ref.stat
A               2.4054E+03  1.0000E+00 3.5061E-06 -5.2219E+04 SER

GAS              Status ENTERED Driving force 0.0000E+00
Moles 2.4054E+03, Mass 2.4054E+04, Volume fraction 1.0000E+00 Mole fractions:
A 1.00000E+00
Constitution:
A 1.00000E+00 A2 8.75433E-20
POLY_3: enter var ha=h;
... the command in full is ENTER_SYMBOL
POLY_3: enter var sa=s;
... the command in full is ENTER_SYMBOL
POLY_3: s-c s
... the command in full is SET_CONDITION
Value /325596.1064/: sa
POLY_3: s-c v=none
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Using already calculated grid

```

```

6 ITS, CPU TIME USED 0 SECONDS
POLY_3: l-e,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:
T=T1, N=2405.43, S=SA
DEGREES OF FREEDOM 0

Temperature 500.00 K ( 226.85 C), Pressure 1.000000E+07
Number of moles of components 2.40543E+03, Mass in grams 2.40543E+04
Total Gibbs energy -1.25610E+08, Enthalpy 3.71880E+07, Volume 1.00000E+00

Component      Moles      M-Fraction Activity Potential Ref.stat
A               2.4054E+03  1.0000E+00 3.5061E-06 -5.2219E+04 SER

GAS
Status ENTERED Driving force 0.0000E+00
Moles 2.4054E+03, Mass 2.4054E+04, Volume fraction 1.0000E+00 Mole fractions:
A 1.00000E+00
Constitution:
A 1.00000E+00 A2 8.75433E-20
POLY_3:Hit RETURN to continue
POLY_3: show t,p,v,g,n,h,s
... the command in full is SHOW_VALUE
T=500
P=1E7
V=1.
G=-1.2561005E8
N=2405.4334
H=3.7188E7
S=325596.11
POLY_3:Hit RETURN to continue
POLY_3: ent var ga=g;
... the command in full is ENTER_SYMBOL
POLY_3: ent var pa=p;
... the command in full is ENTER_SYMBOL
POLY_3: ent var va=v;
... the command in full is ENTER_SYMBOL
POLY_3: @@
POLY_3: @@
POLY_3: save tcex39a y
... the command in full is SAVE_WORKSPACES
POLY_3: s-c t=500
... the command in full is SET_CONDITION
POLY_3: s-c s=204200
... the command in full is SET_CONDITION
POLY_3: s-a-v 1 s 204000 205000,,,
... the command in full is SET_AXIS_VARIABLE
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 137 grid points in 0 s
17 ITS, CPU TIME USED 0 SECONDS
POLY_3: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 204200.
...OK

Phase Region from 204200. for:
GAS
Global test at 2.04400E+05 .... OK
Global test at 2.04650E+05 .... OK
Global test at 2.04900E+05 .... OK
Terminating at 205000.
Calculated 35 equilibria

Phase Region from 204200. for:
GAS
Global test at 2.04000E+05 .... OK
Terminating at 204000.
Calculated 11 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex39a.POLY3
POLY_3: @@
POLY_3: @@
POLY_3: @@ Stage 2. Adiabatic expansion. No heat leaves the system, so the
POLY_3: @@ change in its entropy is zero. In the course of this expansion the
POLY_3: @@ temperature falls from T1 to T2, the temperature of cold reservoir.
POLY_3: @@
POLY_3: s-c s=205000
... the command in full is SET_CONDITION
POLY_3: s-c t=450
... the command in full is SET_CONDITION
POLY_3: s-a-v 1 t 400 500,,,
... the command in full is SET_AXIS_VARIABLE
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 137 grid points in 0 s
13 ITS, CPU TIME USED 0 SECONDS
POLY_3: step norm
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 450.000
...OK

Phase Region from 450.000 for:
GAS
Global test at 4.70000E+02 .... OK
Global test at 4.95000E+02 .... OK
Terminating at 500.000
Calculated 23 equilibria

Phase Region from 450.000 for:
GAS
Global test at 4.30000E+02 .... OK
Global test at 4.05000E+02 .... OK
Terminating at 400.000
Calculated 23 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex

```



```

39a.POLY3
POLY_3: @@
POLY_3: @@ Stage 3. Isothermal compression at T2. The heat Q2 is released to the
POLY_3: @@ cold reservoir, so the change in entropy of the system is -Q2/T2.
POLY_3: @@
POLY_3: s-c t=400
... the command in full is SET_CONDITION
POLY_3: s-c s=204200
... the command in full is SET_CONDITION
POLY_3: s-a-v 1 s 204000 205000,,,
... the command in full is SET_AXIS_VARIABLE
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 137 grid points in 0 s
8 ITS, CPU TIME USED 0 SECONDS
POLY_3: step norm
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 204200.
...OK

Phase Region from 204200. for:
GAS
Global test at 2.04400E+05 .... OK
Global test at 2.04650E+05 .... OK
Global test at 2.04900E+05 .... OK
Terminating at 205000.
Calculated 35 equilibria

Phase Region from 204200. for:
GAS
Global test at 2.04000E+05 .... OK
Terminating at 204000.
Calculated 11 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex
39a.POLY3
POLY_3: @@
POLY_3: @@
POLY_3: @@ Stage 4. Adiabatic compression. No heat enters the system, so the change
POLY_3: @@ in entropy is zero. The temperature rises from T2 to T1.
POLY_3: @@
POLY_3: @@
POLY_3: s-c s=204000
... the command in full is SET_CONDITION
POLY_3: s-c t=450
... the command in full is SET_CONDITION
POLY_3: s-a-v 1 t 400 500,,,
... the command in full is SET_AXIS_VARIABLE
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 137 grid points in 0 s
10 ITS, CPU TIME USED 0 SECONDS
POLY_3: step norm
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 450.000
...OK

Phase Region from 450.000 for:
GAS
Global test at 4.70000E+02 .... OK
Global test at 4.95000E+02 .... OK
Terminating at 500.000
Calculated 23 equilibria

Phase Region from 450.000 for:
GAS
Global test at 4.30000E+02 .... OK
Global test at 4.05000E+02 .... OK
Terminating at 400.000
Calculated 23 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex
39a.POLY3
POLY_3:
POLY_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

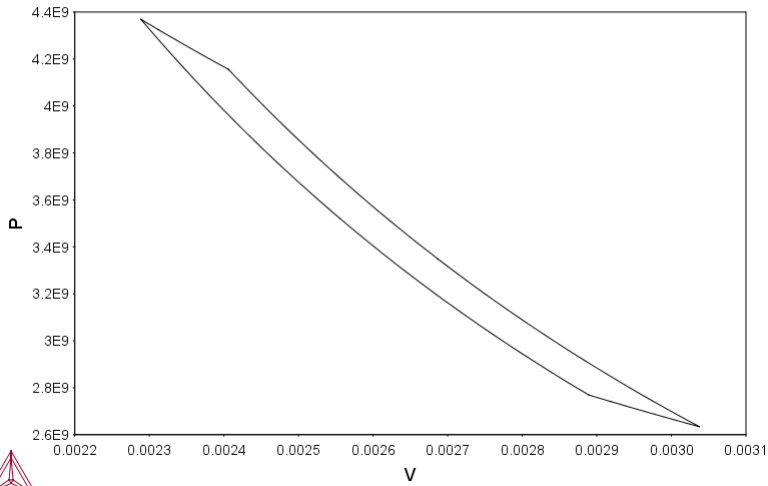
Setting automatic diagram axes

POST:Plotformat
POST:
POST: s-p-f ##1,,,,,,,,,
... the command in full is SET_PLOT_FORMAT
CURRENT DEVICE: TC-UNITE Driver
POST:
POST: s-d-a x v
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y p
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39a
POST: plot
... the command in full is PLOT_DIAGRAM

```

### example 39a

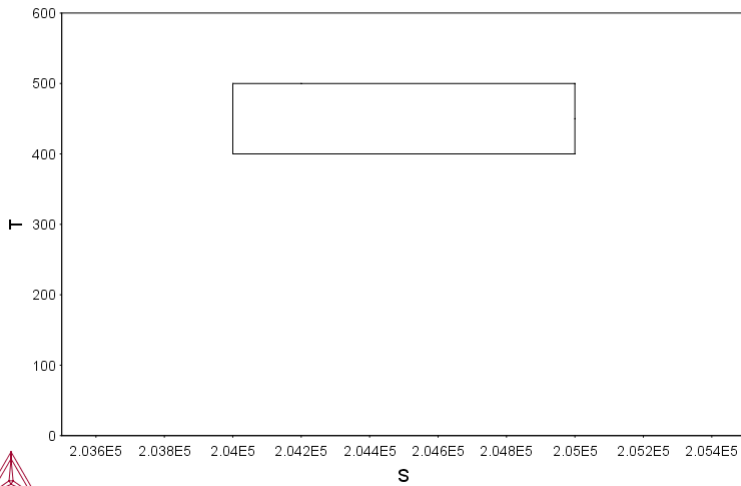
2016.05.16.14.28.57  
User data 2016.05.16: A  
N=2405.43, S=2.04E5



```
POST:
POST:Hit RETURN to continue
POST: @@ The efficiency E of an engine which uses a Carnot cycle is:
POST: @@
POST: @@ E=work performed/heat absorbed = W/Q1
POST: @@ If one plots the entropy versus temperature, one can calculate the
POST: @@ work performed just by calculating the area of the surface
POST: @@ depicted by the two squares and by making the difference between them.
POST: @@
POST: s-d-a x s
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t
... the command in full is SET_DIAGRAM_AXIS
POST: s-s y n 0 600
... the command in full is SET_SCALING_STATUS
POST: s-s x n 203500 205500
... the command in full is SET_SCALING_STATUS
POST: set-title example 39b
POST: plot
... the command in full is PLOT DIAGRAM
```

### example 39b

2016.05.16.14.28.57  
User data 2016.05.16: A  
N=2405.43, S=2.04E5



```
POST:
POST:Hit RETURN to continue
POST: @@
POST: @@
POST: @@ The influence of the value of the temperature T1 (the temperature of the
POST: @@ hot reservoir) on the efficiency of the Carnot cycle is important.
POST: @@ Therefore we will make an other calculation for T1=800 K and compare with
POST: @@ the one for T1=500 K (example 39a and b). T2=400 K in both cases.
POST: ba
... the command in full is BACK
POLY_3: read,,,
... the command in full is READ_WORKSPACES
POLY_3: l-c
... the command in full is LIST_CONDITIONS
T=T1, N=2405.43, S=SA
DEGREES OF FREEDOM 0
POLY_3: s-c s=none
... the command in full is SET_CONDITION
POLY_3: s-c t=800 p=1e7 n=1
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 137 grid points in 0 s
POLY_3: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VXNS/: xn
```

Output from POLY-3, equilibrium = 1, label A0 , database: User dat

Conditions:  
T=800, P=1E7, N=1  
DEGREES OF FREEDOM 0

Temperature 800.00 K ( 526.85 C), Pressure 1.000000E+07  
Number of moles of components 1.00000E+00, Mass in grams 1.00000E+01  
Total Gibbs energy -9.41189E+04, Enthalpy 2.05600E+04, Volume 6.65161E-04

Component	Moles	M-Fraction	Activity	Potential	Ref.stat
A	1.0000E+00	1.0000E+00	7.1585E-07	-9.4119E+04	SER

GAS Status ENTERED Driving force 0.0000E+00  
Moles 1.0000E+00, Mass 1.0000E+01, Volume fraction 1.0000E+00 Mole fractions:  
A 1.00000E+00

Constitution:  
A 1.00000E+00 A2 1.27812E-15

POLY\_3: @@ Set volume to 1 m3

POLY\_3: s-c v

... the command in full is SET\_CONDITION

Value /6.651607999E-04/: 1

POLY\_3: s-c n

... the command in full is SET\_CONDITION

Value /1/: none

POLY\_3: c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Normal POLY minimization, not global

Testing POLY result by global minimization procedure

Using already calculated grid

7 ITS, CPU TIME USED 0 SECONDS

POLY\_3: s-c n

... the command in full is SET\_CONDITION

Value /1503.395871/:

POLY\_3: s-c p

... the command in full is SET\_CONDITION

Value /10000000/: none

POLY\_3: c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Normal POLY minimization, not global

Testing POLY result by global minimization procedure

Using already calculated grid

6 ITS, CPU TIME USED 0 SECONDS

POLY\_3: enter var ha=h;

... the command in full is ENTER\_SYMBOL

POLY\_3: enter var sa=s;

... the command in full is ENTER\_SYMBOL

POLY\_3: s-c s

... the command in full is SET\_CONDITION

Value /215509.7923/: sa

POLY\_3: s-c v=none

... the command in full is SET\_CONDITION

POLY\_3: c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Normal POLY minimization, not global

Testing POLY result by global minimization procedure

Using already calculated grid

6 ITS, CPU TIME USED 0 SECONDS

POLY\_3: show t,p,v,g,n,h,s

... the command in full is SHOW\_VALUE

T=800

P=1E7

V=1.

G=-1.4149801E8

N=1503.3959

H=3.0909819E7

S=215509.79

POLY\_3:Hit RETURN to continue

POLY\_3: save tcex39b y

... the command in full is SAVE\_WORKSPACES

POLY\_3: s-c s=272000

... the command in full is SET\_CONDITION

POLY\_3: s-a-v 1 s 270200 276200,,,

... the command in full is SET\_AXIS\_VARIABLE

POLY\_3: c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Normal POLY minimization, not global

Testing POLY result by global minimization procedure

Calculated 137 grid points in 0 s

53 ITS, CPU TIME USED 0 SECONDS

POLY\_3: step normal

... the command in full is STEP\_WITH\_OPTIONS

No initial equilibrium, using default

Step will start from axis value 272000.

...OK

Phase Region from 272000. for:

GAS

Global test at 2.73200E+05 .... OK

Global test at 2.74700E+05 .... OK

Global test at 2.76200E+05 .... OK

Terminating at 276200.

Calculated 31 equilibria

Phase Region from 272000. for:

GAS

Global test at 2.70800E+05 .... OK

Terminating at 270200.

Calculated 15 equilibria

\*\*\* Buffer saved on file:

c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex

39b.POLY3

POLY\_3: s-c s=276200

... the command in full is SET\_CONDITION

POLY\_3: s-c t=750

... the command in full is SET\_CONDITION

POLY\_3: s-a-v 1 t 400 800,,,

... the command in full is SET\_AXIS\_VARIABLE

POLY\_3: c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Normal POLY minimization, not global

Testing POLY result by global minimization procedure

Calculated 137 grid points in 0 s

13 ITS, CPU TIME USED 0 SECONDS

```

POLY_3: step norm
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value    750.000
...OK

Phase Region from    750.000    for:
GAS
Terminating at      800.000
Calculated          8 equilibria

Phase Region from    750.000    for:
GAS
Global test at      6.70000E+02 .... OK
Global test at      5.70000E+02 .... OK
Global test at      4.70000E+02 .... OK
Terminating at      400.000
Calculated          38 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex
39b.POLY3
POLY_3: s-c t=400
... the command in full is SET_CONDITION
POLY_3: s-c s=270250
... the command in full is SET_CONDITION
POLY_3: s-a-v 1 s 270200 276200,,,
... the command in full is SET_AXIS_VARIABLE
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated          137 grid points in          0 s
          9 ITS, CPU TIME USED    0 SECONDS
POLY_3: step norm
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value    270250.
...OK

Phase Region from    270250.    for:
GAS
Global test at      2.71450E+05 .... OK
Global test at      2.72950E+05 .... OK
Global test at      2.74450E+05 .... OK
Global test at      2.75950E+05 .... OK
Terminating at      276200.
Calculated          43 equilibria

Phase Region from    270250.    for:
GAS
Terminating at      270200.
Calculated          4 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex
39b.POLY3
POLY_3: s-c s=270200
... the command in full is SET_CONDITION
POLY_3: s-c t=750
... the command in full is SET_CONDITION
POLY_3: s-a-v 1 t 400 800,,,
... the command in full is SET_AXIS_VARIABLE
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated          137 grid points in          0 s
          24 ITS, CPU TIME USED    0 SECONDS
POLY_3: step norm
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value    750.000
...OK

Phase Region from    750.000    for:
GAS
Terminating at      800.000
Calculated          8 equilibria

Phase Region from    750.000    for:
GAS
Global test at      6.70000E+02 .... OK
Global test at      5.70000E+02 .... OK
Global test at      4.70000E+02 .... OK
Terminating at      400.000
Calculated          38 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex
39b.POLY3
POLY_3:
POLY_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

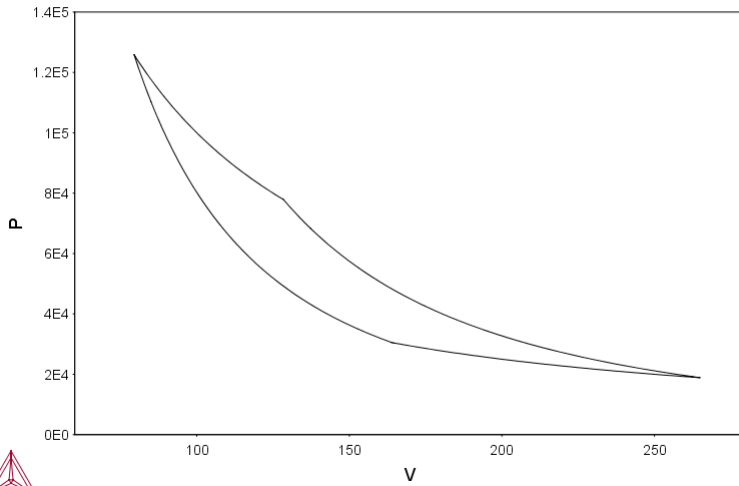
Setting automatic diagram axes

POST: s-p-f ##1,,,,,,,,,
... the command in full is SET_PLOT_FORMAT
CURRENT DEVICE: TC-UNITE Driver
POST:
POST: s-d-a x v
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y p
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39c
POST: plot
... the command in full is PLOT_DIAGRAM

```

# example 39c

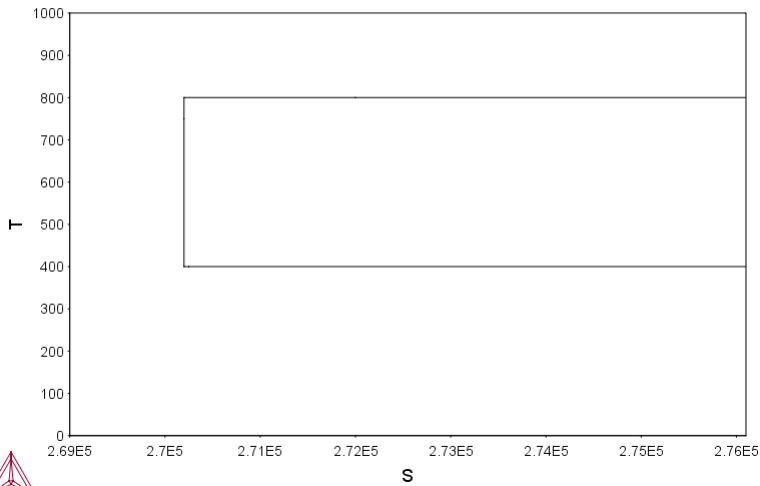
2016.05.16.14.28.58  
User data 2016.05.16: A  
N=1503.4, S=2.702E5



```
POST:
POST:Hit RETURN to continue
POST: s-d-a x s
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y t
... the command in full is SET_DIAGRAM_AXIS
POST: s-s x n 269000 276100
... the command in full is SET_SCALING_STATUS
POST: s-s y n 0 1000
... the command in full is SET_SCALING_STATUS
POST: set-title example 39d
POST: plot
... the command in full is PLOT DIAGRAM
```

## example 39d

2016.05.16.14.28.58  
User data 2016.05.16: A  
N=1503.4, S=2.702E5



```
POST:
POST:Hit RETURN to continue
POST: @@ The efficiency for high value of T1 temperature is almost double compared
POST: @@ with that one for low value of T1 temperature (compare example 39b with
POST: @@ example 39d).
POST: @@
POST: @@ Now we will calculate the Carnot cycle for some real systems. The most
POST: @@ well known engine is the steam engine.
POST: @@
POST: @@ The Carnot cycle for steam engine
POST: @@
POST: ba
... the command in full is BACK
POLY_3: go da
... the command in full is GOTO_MODULE
TDB_TCFE8: rej sys
... the command in full is REJECT
VA DEFINED
L12_FCC B2_BCC B2_VACANCY
HIGH_SIGMA DICTRA_FCC_A1 REJECTED
REINITIATING GES5 .....
TDB_TCFE8: sw subdemo
... the command in full is SWITCH_DATABASE
Current database: Substance Demo Database

VA /- DEFINED
TDB_SUBDEMO: def-sp h2o1
... the command in full is DEFINE_SPECIES
H2O1 DEFINED
TDB_SUBDEMO: l-sys
... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENT/: CONSTITUENTS
GAS:G :H2O1:
H2O1_L :H2O1:
TDB_SUBDEMO: get
```

```

... the command in full is GET_DATA
REINITIATING GES5 .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

'H2O1<G> T.C.R.A.S. Class: 1 H2O1<G> H2O<G> WATER <GAS>, STEAM'
'H2O1<L> T.C.R.A.S. Class: 4 H2O1_Liquid H2O_Liquid Pure Water WATER
T.C.R.A.S. Class: 4 cp modified by atd 12/9/94 and 5/7/2002'
-OK-
TDB_SUBDEMO: @@ patch
TDB_SUBDEMO: go g-e-s
... the command in full is GOTO_MODULE
GIBBS ENERGY SYSTEM version 5.2
GES: li-st,,,,
... the command in full is LIST_STATUS
GAS CONSTANT IN USER ENERGY UNITS:      8.31451000E+00
1 BAR IN USER PRESSURE UNITS:              1.00000000E+05
CURRENT VALUE OF TEMPERATURE (KELVIN):     298.15
CURRENT VALUE OF PRESSURE (PASCAL):        1.00000000E+05

CURRENT NUMBER OF ELEMENT      4

ELEMENT STABLE ELEMENT REFERENCE  MASS      H298-H0      S298
-1 /-  ELECTRON_GAS                0.0000E+00  0.0000E+00  0.0000E+00  80000000
0 VA   VACUUM                      0.0000E+00  0.0000E+00  0.0000E+00  80000000
1 H    1/2_MOLE_H2(GAS)             1.0079E+00  4.2340E+03  6.5285E+01  08000000
2 O    1/2_MOLE_O2(GAS)             1.5999E+01  4.3410E+03  1.0252E+02  08000000

CURRENT NUMBER OF PHASE      2

PHASE      STATUS  SUBLATTICES
1 GAS      88200000  1
2 H2O1_L   82200000  1

CURRENT NUMBER OF SPECIES    4

SPECIES      STOICHIOMETRY
1 H          80800000  H
2 H2O1       00000000  H2O1
3 O          80800000  O
4 VA         81800000  VA

GES: @@ patch
GES: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3: l-st
... the command in full is LIST_STATUS
Option /CPS/: CPS
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS  REF. STATE  T(K)      P(Pa)
VA             ENTERED  SER
H             ENTERED  SER
O             ENTERED  SER
*** STATUS FOR ALL PHASES
PHASE          STATUS  DRIVING FORCE  MOLES
H2O1_L         ENTERED  0.000000E+00  0.000000E+00
GAS            ENTERED  0.000000E+00  0.000000E+00
*** STATUS FOR ALL SPECIES
H ENTERED  H2O1 ENTERED  O ENTERED  VA ENTERED
POLY_3: c-st p h2o_l=sus
... the command in full is CHANGE_STATUS
POLY_3: l-st
... the command in full is LIST_STATUS
Option /CPS/: CPS
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS  REF. STATE  T(K)      P(Pa)
VA             ENTERED  SER
H             ENTERED  SER
O             ENTERED  SER
*** STATUS FOR ALL PHASES
PHASE          STATUS  DRIVING FORCE  MOLES
GAS            ENTERED  0.000000E+00  0.000000E+00
SUSPENDED PHASES:
H2O1_L
*** STATUS FOR ALL SPECIES
H ENTERED  H2O1 ENTERED  O ENTERED  VA ENTERED
POLY_3: @@ The Carnot cycle will be calculated for T1=350 K and T2=450 K
POLY_3: @@
POLY_3: s-c t=380 p=1e5 n=100 ac(o)=1
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated      1 grid points in      0 s
6 ITS, CPU TIME USED 0 SECONDS
POLY_3: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VXNS/: xn
Output from POLY-3, equilibrium =      1, label A0 , database: SUBDEMO

Conditions:
T=380, P=1E5, N=100, AC(O)=1
DEGREES OF FREEDOM 0

Temperature 380.00 K ( 106.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+02, Mass in grams 6.00493E+02
Total Gibbs energy -1.04643E+07, Enthalpy -7.96861E+06, Volume 1.05317E+00

Component      Moles      M-Fraction  Activity  Potential  Ref.stat
H              6.6667E+01  6.6667E-01  2.6556E-22 -1.5697E+05 SER
O              3.3333E+01  3.3333E-01  1.0000E+00  0.0000E+00 SER

GAS            Status ENTERED      Driving force 0.0000E+00
Moles 1.0000E+02, Mass 6.0049E+02, Volume fraction 1.0000E+00 Mole fractions:
H 6.66667E-01 O 3.33333E-01
Constitution:

```

```

H2O1 1.00000E+00
POLY_3: s-c p=none
... the command in full is SET_CONDITION
POLY_3: s-c s
... the command in full is SET_CONDITION
Value /6567.729231/: 6100
POLY_3: s-c t=350
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 1 grid points in 0 s
10 ITS, CPU TIME USED 0 SECONDS
POLY_3: l-e,,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: SUBDEMO

Conditions:
T=350, N=100, AC(O)=1, S=6100
DEGREES OF FREEDOM 0

Temperature 350.00 K ( 76.85 C), Pressure 3.863619E+05
Number of moles of components 1.00000E+02, Mass in grams 6.00493E+02
Total Gibbs energy -1.01376E+07, Enthalpy -8.00259E+06, Volume 2.51067E-01

Component      Moles      M-Fraction  Activity  Potential  Ref.stat
H               6.6667E+01  6.6667E-01  2.0244E-23 -1.5206E+05 SER
O               3.3333E+01  3.3333E-01  1.0000E+00  0.0000E+00 SER

GAS              Status ENTERED   Driving force  0.0000E+00
Moles 1.0000E+02, Mass 6.0049E+02, Volume fraction 1.0000E+00 Mole fractions:
H 6.66667E-01 O 3.33333E-01
Constitution:
H2O1 1.00000E+00
POLY_3: @@ step in S with t=350
POLY_3: s-a-v 1 s 6000 7000,,,,
... the command in full is SET_AXIS_VARIABLE
POLY_3: save tcex39c y
... the command in full is SAVE_WORKSPACES
POLY_3: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 6100.00
...OK

Phase Region from 6100.00 for:
GAS
Global test at 6.30000E+03 .... OK
Global test at 6.55000E+03 .... OK
Global test at 6.80000E+03 .... OK
Terminating at 7000.00
Calculated 39 equilibria

Phase Region from 6100.00 for:
GAS
Terminating at 6000.00
Calculated 7 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex
39c.POLY3
POLY_3:
POLY_3:
POLY_3: read,,,,
... the command in full is READ_WORKSPACES
POLY_3: s-c s=6000
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 1 grid points in 0 s
8 ITS, CPU TIME USED 0 SECONDS
POLY_3: @@ step in T with S=6000
POLY_3: s-a-v 1 t 350 450,,,,
... the command in full is SET_AXIS_VARIABLE
POLY_3: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 350.000
...OK

Phase Region from 350.000 for:
GAS
Global test at 3.70000E+02 .... OK
Global test at 3.95000E+02 .... OK
Global test at 4.20000E+02 .... OK
Global test at 4.45000E+02 .... OK
Terminating at 450.000
Calculated 43 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex
39c.POLY3
POLY_3:
POLY_3: read,,,,
... the command in full is READ_WORKSPACES
POLY_3: s-c t=450
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 1 grid points in 0 s
9 ITS, CPU TIME USED 0 SECONDS
POLY_3: @@ Step in S with t=450
POLY_3: @@@@
POLY_3: s-a-v 1 s 6000 7000,,,,
... the command in full is SET_AXIS_VARIABLE
POLY_3: step norm
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 6100.00
...OK

```

```

Phase Region from 6100.00 for:
  GAS
Global test at 6.30000E+03 .... OK
Global test at 6.55000E+03 .... OK
Global test at 6.80000E+03 .... OK
Terminating at 7000.00
Calculated 39 equilibria

Phase Region from 6100.00 for:
  GAS
Terminating at 6000.00
Calculated 7 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex
39c.POLY3
POLY_3:
POLY_3: s-c s=7000
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated 1 grid points in 0 s
42 ITS, CPU TIME USED 0 SECONDS
POLY_3: @@ Step in T with S=7000
POLY_3: s-a-v 1 t 350 450,,,
... the command in full is SET_AXIS_VARIABLE
POLY_3: step norm
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 450.000
...OK

Phase Region from 450.000 for:
  GAS
Global test at 4.30000E+02 .... OK
Global test at 4.05000E+02 .... OK
Global test at 3.80000E+02 .... OK
Global test at 3.55000E+02 .... OK
Terminating at 350.000
Calculated 43 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex
39c.POLY3
POLY_3:
POLY_3: post

```

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

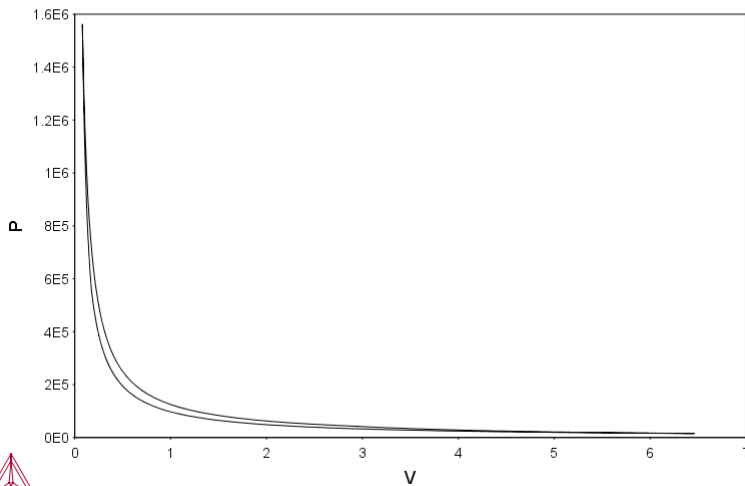
```

POST: s-p-f ##1,,,,,,,,
... the command in full is SET_PLOT_FORMAT
CURRENT DEVICE: TC-UNITE Driver
POST:
POST: s-d-a x v
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y p
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39e
POST: plot
... the command in full is PLOT DIAGRAM

```

**example 39e**

2016.05.16.14.29.00  
SUBDEMO: H<sub>2</sub>O  
N=100, AC(O)=1, S=7000.



```

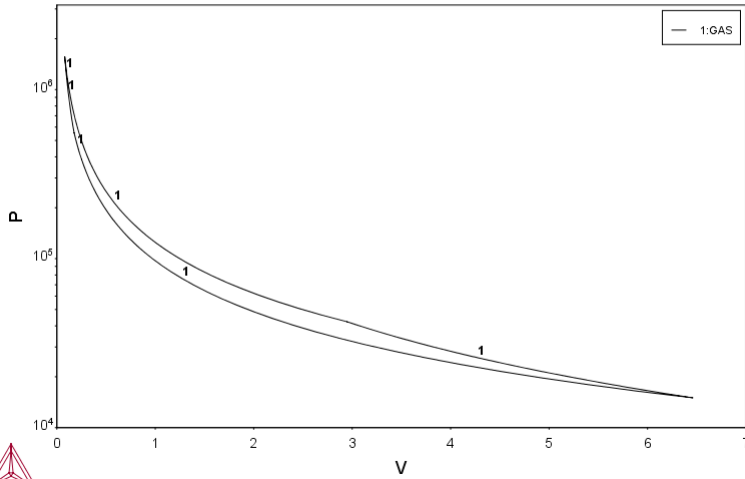
POST:
POST:Hit RETURN to continue
POST: s-a-ty y log
... the command in full is SET_AXIS_TYPE
POST: s-lab b
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 39f
POST: plot
... the command in full is PLOT_DIAGRAM

```



# example 39f

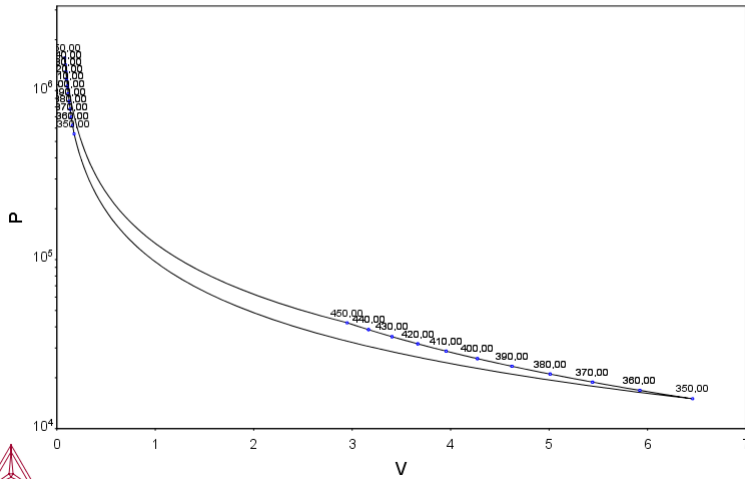
2016.05.16.14.29.00  
SUBDEMO: H, O  
N=100, AC(O)=1, S=7000.



```
POST:
POST:Hit RETURN to continue
POST: @@ It is a bit difficult to distinguish from the calculated diagram,
POST: @@ example 39e, where the adiabatic expansion and compression start.
POST: @@ Therefore it is good to plot on the same diagram also the temperature.
POST: @@
POST: s-d-a z t
... the command in full is SET_DIAGRAM_AXIS
POST: s-lab none
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 39g
POST: plot
... the command in full is PLOT DIAGRAM
```

# example 39g

2016.05.16.14.29.00  
SUBDEMO: H, O  
N=100, AC(O)=1, S=7000.



```
POST:
POST:Hit RETURN to continue
POST: @@
POST: @@ With Thermo-Calc one may also calculate the Carnot cycle for real systems
POST: @@ and also include phase transformations.
POST: @@
POST: @@ Trying a Carnot cycle for water - it shows the case with H2O_liquid
POST: @@ to gas phase transformation. In the calculations the volum of the liquid
POST: @@ water was ignored.
POST: @@
POST: ba
... the command in full is BACK
POLY_3: go da
... the command in full is GOTO_MODULE
TDB_SUBDEMO: rej sys
... the command in full is REJECT
VA /- DEFINED
REINITIATING GES5 .....
TDB_SUBDEMO: sw subdemo
... the command in full is SWITCH_DATABASE
TDB_SUBDEMO: def-sp h2o1
... the command in full is DEFINE_SPECIES
H2O1 DEFINED
TDB_SUBDEMO: l-sys
... the command in full is LIST_SYSTEM
ELEMENTS, SPECIES, PHASES OR CONSTITUENTS: /CONSTITUENTS/: CONSTITUENTS
GAS:G :H2O1:
H2O1 L :H2O1:
TDB_SUBDEMO: get
... the command in full is GET_DATA
REINITIATING GES5 .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
```

FUNCTIONS ....

List of references for assessed data

'H2O1<G> T.C.R.A.S. Class: 1 H2O1<G> H2O<G> WATER <GAS>, STEAM'  
'H2O1<L> T.C.R.A.S. Class: 4 H2O1\_Liquid H2O\_Liquid Pure Water WATER  
T.C.R.A.S. Class: 4 cp modified by atd 12/9/94 and 5/7/2002'

-OK-

**TDB SUBDEMO:** @@ patch

**TDB SUBDEMO:** go g-e-s

... the command in full is GOTO\_MODULE

GIBBS ENERGY SYSTEM version 5.2

**GES:** li-st,,,,,

... the command in full is LIST\_STATUS

GAS CONSTANT IN USER ENERGY UNITS: 8.31451000E+00

1 BAR IN USER PRESSURE UNITS: 1.00000000E+05

CURRENT VALUE OF TEMPERATURE (KELVIN): 298.15

CURRENT VALUE OF PRESSURE (PASCAL): 1.00000000E+05

CURRENT NUMBER OF ELEMENT 4

ELEMENT	STABLE ELEMENT REFERENCE	MASS	H298-H0	S298
-1 /-	ELECTRON_GAS	0.0000E+00	0.0000E+00	0.0000E+00 80000000
0 VA	VACUUM	0.0000E+00	0.0000E+00	0.0000E+00 80000000
1 H	1/2_MOLE_H2(GAS)	1.0079E+00	4.2340E+03	6.5285E+01 08000000
2 O	1/2_MOLE_O2(GAS)	1.5999E+01	4.3410E+03	1.0252E+02 08000000

CURRENT NUMBER OF PHASE 2

PHASE	STATUS	SUBLATTICES
1 GAS	88200000	1
2 H2O1_L	82200000	1

CURRENT NUMBER OF SPECIES 4

SPECIES	STOICHIOMETRY
1 H	80800000 H
2 H2O1	00000000 H2O1
3 O	80800000 O
4 VA	81800000 VA

**GES:** @@ patch

**GES:** go p-3

... the command in full is GOTO\_MODULE

POLY version 3.32

**POLY\_3:** l-st

... the command in full is LIST\_STATUS

**Option /CPS/:** CPS

\*\*\* STATUS FOR ALL COMPONENTS

COMPONENT	STATUS	REF. STATE	T(K)	P(Pa)
VA	ENTERED	SER		
H	ENTERED	SER		
O	ENTERED	SER		

\*\*\* STATUS FOR ALL PHASES

PHASE	STATUS	DRIVING FORCE	MOLES
H2O1_L	ENTERED	0.000000E+00	0.000000E+00
GAS	ENTERED	0.000000E+00	0.000000E+00

\*\*\* STATUS FOR ALL SPECIES

H	ENTERED	H2O1	ENTERED	O	ENTERED	VA	ENTERED
---	---------	------	---------	---	---------	----	---------

**POLY\_3:** c-st p h2o\_l=e 0

... the command in full is CHANGE\_STATUS

**POLY\_3:** l-st

... the command in full is LIST\_STATUS

**Option /CPS/:** CPS

\*\*\* STATUS FOR ALL COMPONENTS

COMPONENT	STATUS	REF. STATE	T(K)	P(Pa)
VA	ENTERED	SER		
H	ENTERED	SER		
O	ENTERED	SER		

\*\*\* STATUS FOR ALL PHASES

PHASE	STATUS	DRIVING FORCE	MOLES
H2O1_L	ENTERED	0.000000E+00	0.000000E+00
GAS	ENTERED	0.000000E+00	0.000000E+00

\*\*\* STATUS FOR ALL SPECIES

H	ENTERED	H2O1	ENTERED	O	ENTERED	VA	ENTERED
---	---------	------	---------	---	---------	----	---------

**POLY\_3:** s-c t=380 p=1e5 n=100 ac(o)=1

... the command in full is SET\_CONDITION

**POLY\_3:** l-c

... the command in full is LIST\_CONDITIONS

T=380, P=1E5, N=100, AC(O)=1

DEGREES OF FREEDOM 0

**POLY\_3:** c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Normal POLY minimization, not global

Testing POLY result by global minimization procedure

Calculated 2 grid points in 0 s

6 ITS, CPU TIME USED 0 SECONDS

**POLY\_3:** l-e

... the command in full is LIST\_EQUILIBRIUM

**OUTPUT TO SCREEN OR FILE /SCREEN/:**

**Options /VXNS/:** xn

Output from POLY-3, equilibrium = 1, label A0 , database: SUBDEMO

Conditions:

T=380, P=1E5, N=100, AC(O)=1

DEGREES OF FREEDOM 0

Temperature 380.00 K ( 106.85 C), Pressure 1.000000E+05

Number of moles of components 1.00000E+02, Mass in grams 6.00493E+02

Total Gibbs energy -1.04643E+07, Enthalpy -7.96861E+06, Volume 1.05317E+00

Component	Moles	M-Fraction	Activity	Potential	Ref.stat
H	6.6667E+01	6.6667E-01	2.6556E-22	-1.5697E+05	SER
O	3.3333E+01	3.3333E-01	1.0000E+00	0.0000E+00	SER

GAS Status ENTERED Driving force 0.0000E+00

Moles 1.0000E+02, Mass 6.0049E+02, Volume fraction 1.0000E+00 Mole fractions:

H 6.66667E-01 O 3.33333E-01

Constitution:

H2O1 1.00000E+00

**POLY\_3:** s-c p=none

... the command in full is SET\_CONDITION

**POLY\_3:** s-c s

... the command in full is SET\_CONDITION

```

Value /6567.729231/: 6100
POLY_3: s-c t=350
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated      2 grid points in      0 s
36 ITS, CPU TIME USED  0 SECONDS
POLY_3: l-e,,,,
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: SUBDEMO

Conditions:
T=350, N=100, AC(0)=1, S=6100
DEGREES OF FREEDOM 0

Temperature 350.00 K ( 76.85 C), Pressure 4.130269E+04
Number of moles of components 1.00000E+02, Mass in grams 6.00493E+02
Total Gibbs energy -1.03545E+07, Enthalpy -8.21947E+06, Volume 1.98337E+00

Component      Moles      M-Fraction Activity Potential Ref.stat
H               6.6667E+01  6.6667E-01 6.6188E-24 -1.5532E+05 SER
O               3.3333E+01  3.3333E-01 1.0000E+00  0.0000E+00 SER

GAS              Status ENTERED      Driving force 0.0000E+00
Moles 8.4450E+01, Mass 5.0711E+02, Volume fraction 1.0000E+00 Mole fractions:
H 6.66667E-01 O 3.33333E-01
Constitution:
H2O1 1.00000E+00

H2O1_L           Status ENTERED      Driving force 0.0000E+00
Moles 1.5550E+01, Mass 9.3379E+01, Volume fraction 0.0000E+00 Mole fractions:
H 6.66667E-01 O 3.33333E-01
Constitution:
H2O1 1.00000E+00
POLY_3: @@ step in S with t=350
POLY_3: s-a-v 1 s 6000 7000,,,,
... the command in full is SET_AXIS_VARIABLE
POLY_3: save tcex39d y
... the command in full is SAVE_WORKSPACES
POLY_3: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 6100.00
...OK

Phase Region from 6100.00 for:
GAS
H2O1_L
Global test at 6.30000E+03 .... OK
Global test at 6.55000E+03 .... OK
Global check of removing phase at 6.71967E+03
Calculated 27 equilibria

Phase Region from 6719.67 for:
GAS
Global test at 6.90000E+03 .... OK
Terminating at 7000.00
Calculated 15 equilibria

Phase Region from 6100.00 for:
GAS
H2O1_L
Terminating at 6000.00
Calculated 7 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex
39d.POLY3
POLY_3:
POLY_3: read,,,,
... the command in full is READ_WORKSPACES
POLY_3: s-c s=6000
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated      2 grid points in      0 s
6 ITS, CPU TIME USED  0 SECONDS
POLY_3: @@ step in T with S=6000
POLY_3: s-a-v 1 t 350 450,,,
... the command in full is SET_AXIS_VARIABLE
POLY_3: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 350.000
...OK

Phase Region from 350.000 for:
GAS
H2O1_L
Global test at 3.70000E+02 .... OK
Global test at 3.95000E+02 .... OK
Global test at 4.20000E+02 .... OK
Global test at 4.45000E+02 .... OK
Terminating at 450.000
Calculated 43 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex
39d.POLY3
POLY_3:
POLY_3: read,,,,
... the command in full is READ_WORKSPACES
POLY_3: s-c t=450
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated      2 grid points in      0 s
12 ITS, CPU TIME USED  0 SECONDS
POLY_3: @@ Step in S with t=450
POLY_3: @@
POLY_3: s-a-v 1 s 6000 7000,,,,

```

```

... the command in full is SET_AXIS_VARIABLE
POLY_3: step norm
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value    6100.00
...OK

Phase Region from    6100.00    for:
  GAS
  H2O1_L
Global check of removing phase at  6.16203E+03
Calculated    5 equilibria

Phase Region from    6162.03    for:
  GAS
Global test at   6.35000E+03 .... OK
Global test at   6.60000E+03 .... OK
Global test at   6.85000E+03 .... OK
Terminating at    7000.00
Calculated    37 equilibria

Phase Region from    6100.00    for:
  GAS
  H2O1_L
Terminating at    6000.00
Calculated    7 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex
39d.POLY3
POLY_3:
POLY_3: s-c s=7000
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Calculated    2 grid points in    0 s
  40 ITS, CPU TIME USED    0 SECONDS
POLY_3: @@ Step in T with S=7000
POLY_3: s-a-v 1 t 350 450,,,
... the command in full is SET_AXIS_VARIABLE
POLY_3: step norm
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value    450.000
...OK

Phase Region from    450.000    for:
  GAS
Global test at   4.30000E+02 .... OK
Global test at   4.05000E+02 .... OK
Global test at   3.80000E+02 .... OK
Global test at   3.55000E+02 .... OK
Terminating at    350.000
Calculated    43 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex39\tcex
39d.POLY3
POLY_3:
POLY_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

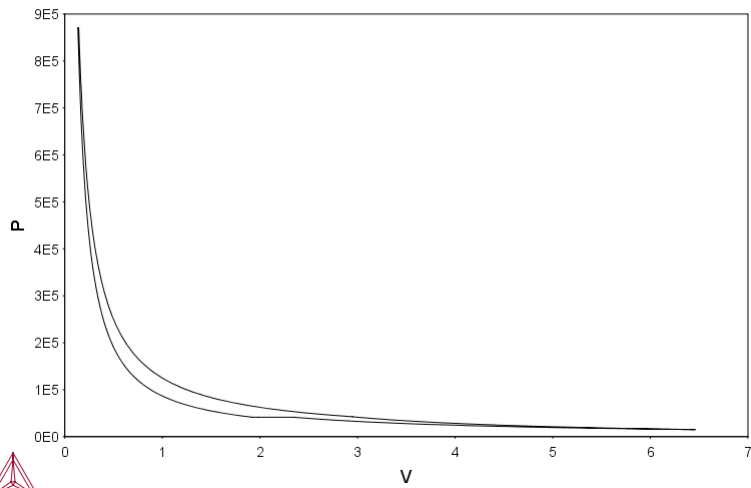
Setting automatic diagram axes

POST: @@ The cycle shows the constant pressure at phase transformation.
POST: s-p-f ##1,,,,,,,,,
... the command in full is SET_PLOT_FORMAT
CURRENT DEVICE: TC-UNITE Driver
POST:
POST: @@ To get a better understanding of this process it is now possible to plot
POST: @@ the cycle using any set of thermodynamic state variables.
POST: @@ Thus, from the pressure-volume-temperature diagram, example 39g, it is
POST: @@ possible to see the temperature variation on the two adiabatical stages
POST: @@ of the Carnot cycle.
POST: @@ The cycle shows the constant pressure at phase transformation.
POST: s-d-a x v
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y p
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39h
POST: plot
... the command in full is PLOT_DIAGRAM

```

# example 39h

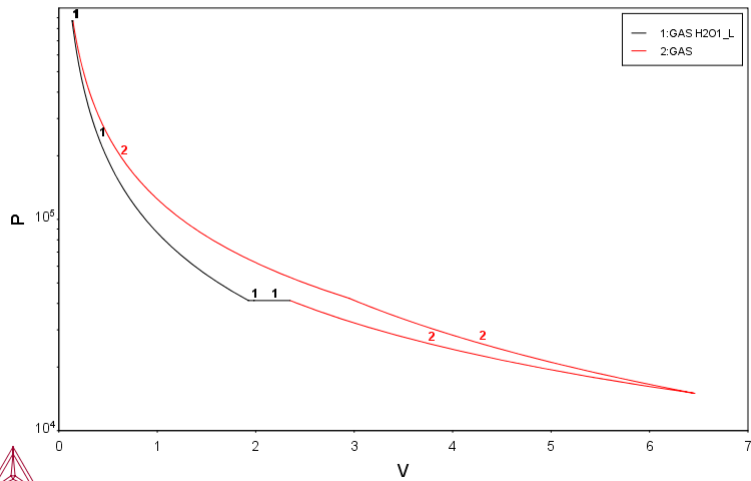
2016.05.16.14.29.01  
SUBDEMO: H, O  
N=100, AC(O)=1, S=7000



POST:  
POST:Hit RETURN to continue  
POST: s-a-ty y log  
... the command in full is SET\_AXIS\_TYPE  
POST: s-lab b  
... the command in full is SET\_LABEL\_CURVE\_OPTION  
POST: s-tit example 39i  
... the command in full is SET\_TITLE  
POST: plot  
... the command in full is PLOT DIAGRAM

## example 39i

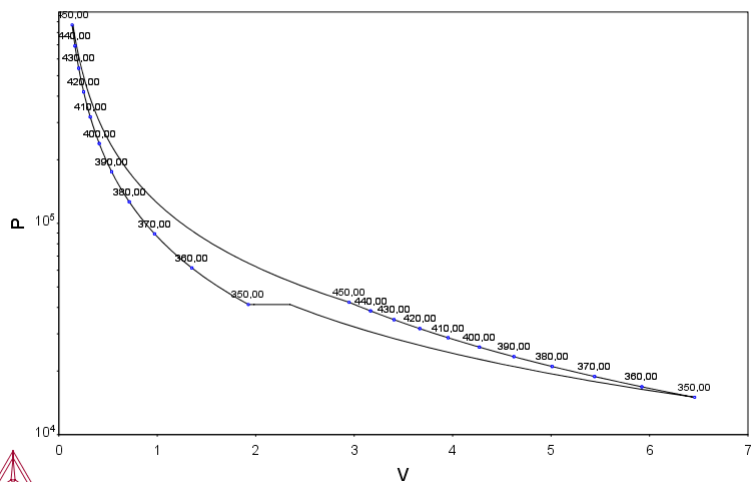
2016.05.16.14.29.02  
SUBDEMO: H, O  
N=100, AC(O)=1, S=7000



POST:  
POST:Hit RETURN to continue  
POST: s-d-a z t  
... the command in full is SET\_DIAGRAM\_AXIS  
POST: s-lab none  
... the command in full is SET\_LABEL\_CURVE\_OPTION  
POST: set-title example 39j  
POST: plot  
... the command in full is PLOT\_DIAGRAM

### example 39j

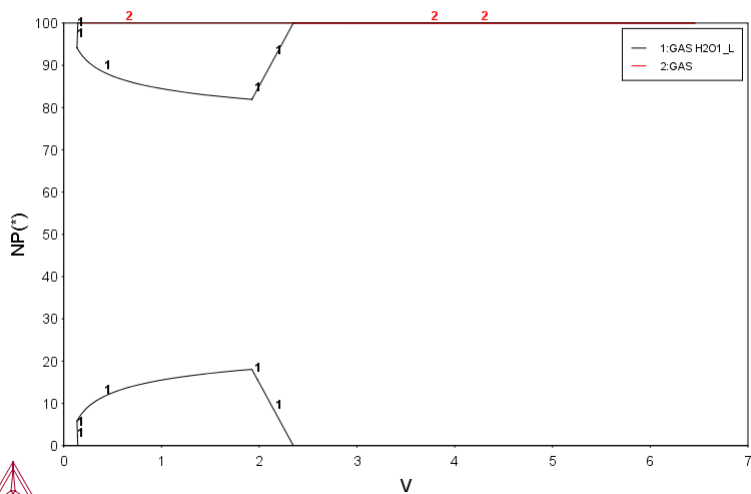
2016.05.16.14.29.02  
SUBDEMO: H, O  
N=100, AC(O)=1, S=7000



```
POST:
POST:Hit RETURN to continue
POST: @@ Also interesting seems to plot the amount of phases versus volume. One
POST: @@ could get information about both the kind and amount of phases which
POST: @@ fill up a certain volume.
POST: s-d-a z none
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y np(*),,,
... the command in full is SET_DIAGRAM_AXIS
POST: s-a-ty Y,,,
... the command in full is SET_AXIS_TYPE
POST: s-lab b
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 39k
POST: plot
... the command in full is PLOT_DIAGRAM
```

### example 39k

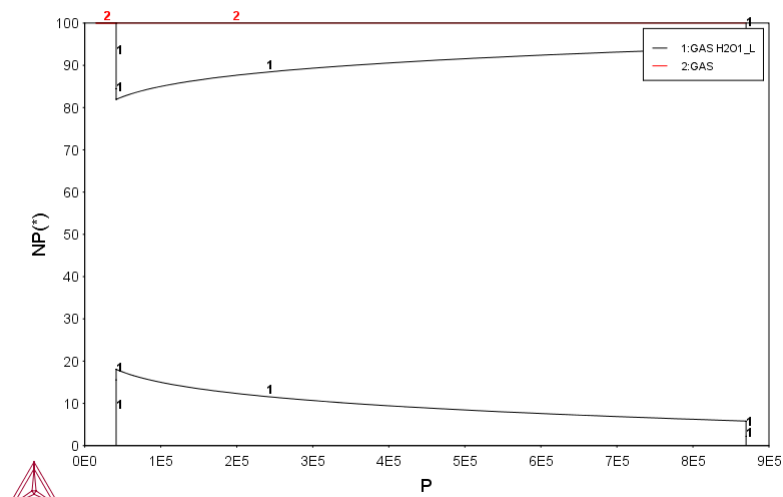
2016.05.16.14.29.02  
SUBDEMO: H, O  
N=100, AC(O)=1, S=7000



```
POST:
POST:Hit RETURN to continue
POST: @@ Next diagram shows the amount of phases versus pressure. It gives important
POST: @@ information on the phase transformation pressure and on the ratio
POST: @@ between the two phases in equilibrium at a certain pressure.
POST: @@
POST: s-d-a x p
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 39l
POST: plot
... the command in full is PLOT_DIAGRAM
```

# example 39l

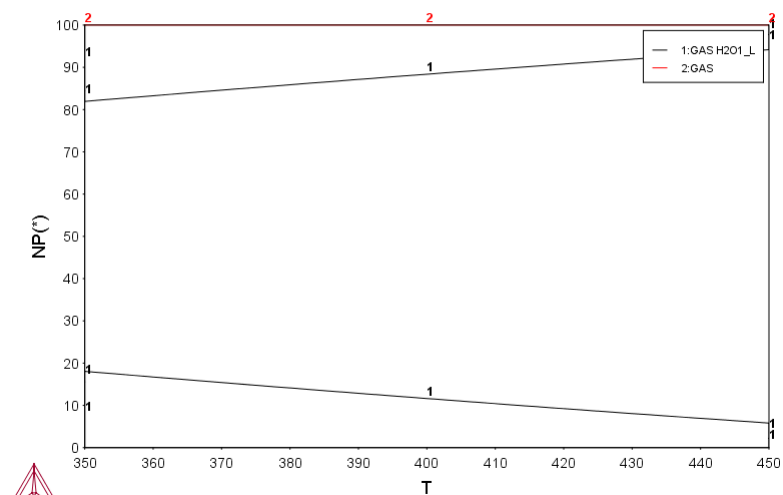
2016.05.16.14.29.02  
SUBDEMO: H, O  
N=100, AC(O)=1, S=7000



POST:  
POST:Hit RETURN to continue  
POST: @@ By plotting the amount of phases versus temperature, example 39k, it is  
POST: @@ possible to know the phase transformation temperature and also the ratio  
POST: @@ between the two phases in equilibrium at a certain temperature.  
POST: @@  
POST: s-d-a x t  
... the command in full is SET\_DIAGRAM\_AXIS  
POST: set-title example 39m  
POST: plot  
... the command in full is PLOT DIAGRAM

## example 39m

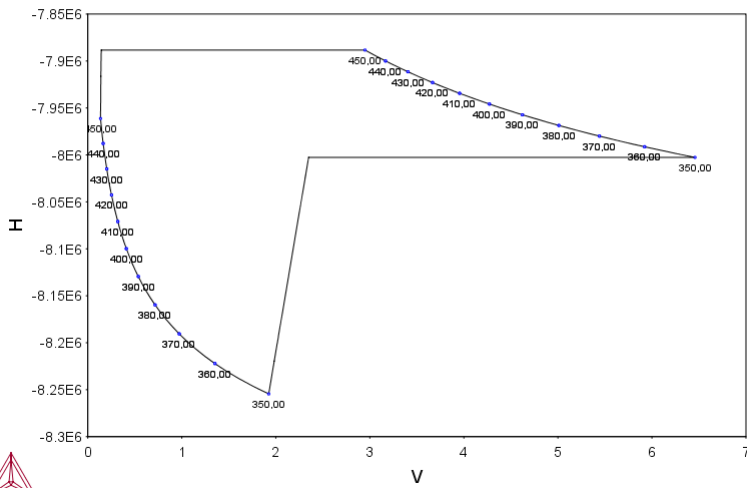
2016.05.16.14.29.03  
SUBDEMO: H, O  
N=100, AC(O)=1, S=7000



POST:  
POST:Hit RETURN to continue  
POST: @@ The enthalpy and Gibbs energy for the Carnot cycle could also be  
POST: @@ plotted using the same calculation but a different set for diagram axis.  
POST: @@ Note the important drop of the enthalpy at the phase transformation  
POST: @@ point, example 39l.  
POST: s-lab none  
... the command in full is SET\_LABEL\_CURVE\_OPTION  
POST: s-d-a x v  
... the command in full is SET\_DIAGRAM\_AXIS  
POST: s-d-a y h  
... the command in full is SET\_DIAGRAM\_AXIS  
POST: s-d-a z t  
... the command in full is SET\_DIAGRAM\_AXIS  
POST: set-title example 39n  
POST: plot  
... the command in full is PLOT\_DIAGRAM

# example 39n

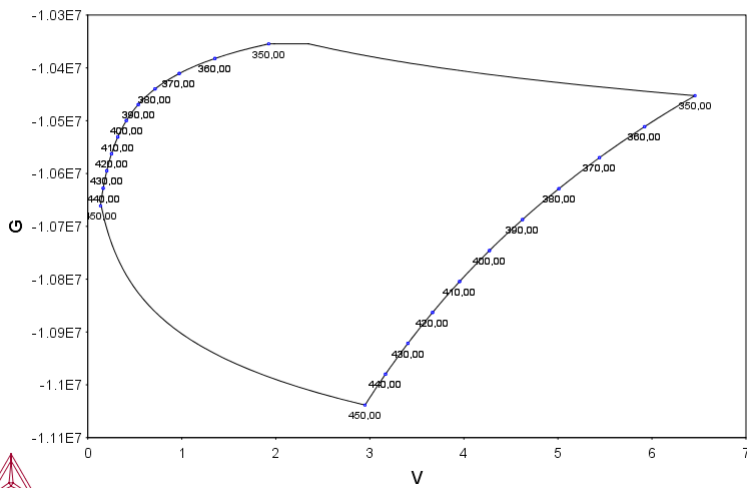
2016.05.16.14.29.03  
SUBDEMO: H, O  
N=100, AC(O)=1, S=7000



POST:  
POST:Hit RETURN to continue  
POST: s-d-a x v  
... the command in full is SET\_DIAGRAM\_AXIS  
POST: s-d-a y g  
... the command in full is SET\_DIAGRAM\_AXIS  
POST: set-title example 39o  
POST: plot  
... the command in full is PLOT DIAGRAM

# example 39o

2016.05.16.14.29.03  
SUBDEMO: H, O  
N=100, AC(O)=1, S=7000



POST:  
POST:Hit RETURN to continue  
POST: set-inter  
... the command in full is SET\_INTERACTIVE\_MODE  
POST:



## tcex40-TCEX40

### About Stockholm, Sweden

Software (build 9597) running on WinNT 64-bit wordlength  
Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118  
License library version: 8.5.1.0017  
Linked: Tue May 17 19:06:04 2016

**SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex40\TCEX40.TCM"SYS:**

**SYS:SYS:** set-echo

**SYS:**

**SYS:** set-log TCEX40.LOG

**Heading:** Pourbaix Diagram Calculations through the advanced POURBAIX module

**SYS:**

**SYS:** @@

**SYS:** @@ TCEX40: Thermo-Calc 4.0 (Console Mode) Standard Example No 40

**SYS:** @@ \*\*\*\*\* =====

**SYS:** @@ Copyright: Thermo-Calc Software AB, Stockholm, Sweden

**SYS:** @@ Developer: Dr. Pingfang Shi, Thermo-Calc Software AB

**SYS:** @@ Date: 2014-05-18 (revision)

**SYS:** @@

**SYS:** @@ Pourbaix Diagram Calculations through the advanced POURBAIX module

**SYS:** @@ \*\*\*\*\* =====

**SYS:** @@ \* Using PAQ2 or PAQS2 database;

**SYS:** @@ \* For the Fe-H2O-NaCl heterogeneous interaction systems

**SYS:** @@

**SYS:** @@ List of all the TC4-CM\_Ex40 examples related to the POURBAIX module:

**SYS:** @@ -----

**SYS:** @@ TCEX40:

**SYS:** @@ \* With the Main Option 1

**SYS:** @@ \* Using the Single-Database Option, i.e., retrieving data from

**SYS:** @@ the PAQ2 [TCS Public Aqueous Solution (SIT) Database, v2.4;

**SYS:** @@ using the SIT aqueous solution model] or PAQS2 [TCS Public

**SYS:** @@ Aqueous Solution Database, v2.4; using the Complete Revised

**SYS:** @@ HKF aqueous solution model]; both of which contain an AQUEOUS

**SYS:** @@ solution phase and REF\_ELECTRODE phase (as a reference for

**SYS:** @@ electron in aqueous electrolyte systems), as well as some

**SYS:** @@ data for various solid phases (solution or stoichiometric)

**SYS:** @@ and gaseous mixture phase. The PAQ2 and PAQS2 are specially

**SYS:** @@ designed for demonstrations of calculations of the so-called

**SYS:** @@ Pourbaix diagrams (i.e., pH-Eh plots) and other types of

**SYS:** @@ phase diagrams or property diagrams in some aqueous-bearing

**SYS:** @@ multicomponent heterogeneous interaction systems within the

**SYS:** @@ limited chemical framework of Fe-Co-Cr-Ni-C-N-S-H2O-NaCl,

**SYS:** @@ via the Single-Database Option in the advanced POURBAIX

**SYS:** @@ module or through the normal TDB-GES-PLOY-POST routine.

**SYS:** @@ \* By reading a saved POURBAIX.POLY3 file (or renamed as another

**SYS:** @@ name), one can further run the following Main Options:

**SYS:** @@ Main Option 2 for plotting many other property diagrams

**SYS:** @@ of the calculated interaction system;

**SYS:** @@ Main Option 3 for making another POURBAIX calculation

**SYS:** @@ of the same chemical system but under

**SYS:** @@ a different P-T-X condition;

**SYS:** @@ Main Option 4 for making a POLY3 STEPPING calculation

**SYS:** @@ of the same chemical system but varied

**SYS:** @@ with only one independent variable;

**SYS:** @@ \*\* The Main Options 2, 3 and 4 are not illustrated in this

**SYS:** @@ TCEX40 example.

**SYS:** @@

**SYS:** @@ Note that five more examples (TCEX40A, TCEX40B, TCEX40C, TCEX40D

**SYS:** @@ and TCEX40E) are also provided to demonstrate various options

**SYS:** @@ and features in the POURBAIX module and to show more advanced

**SYS:** @@ applications of the TCAQ2 and AQS2 aqueous solution databases

**SYS:** @@ [in the Multiple-Database Option, i.e., with appended data

**SYS:** @@ from the SSOL5 and SSUB5 databases].

**SYS:** @@

**SYS:** @@ -----

**SYS:** @@ In this Standard Example (TCEX40):

**SYS:** @@ =====

**SYS:** @@ The Pourbaix diagram for 0.001 m Fe in a 0.1 m NaCl aqueous

**SYS:** @@ solution at 25C and 1 bar is automatically calculated and

**SYS:** @@ plotted.

**SYS:** @@

**SYS:** @@ A so-called Pourbaix diagram is actually a phase diagram with

**SYS:** @@ independently-varied acidity (pH) and electropotential (Eh),

**SYS:** @@ for a heterogeneous interaction system at a certain bulk

**SYS:** @@ composition (that is by default always set as 1 kg of water

**SYS:** @@ dissolving a specified amount of metals and other solutes),

**SYS:** @@ under a defined temperature and pressure condition.

**SYS:** @@

**SYS:** @@ Some other diagrams, along various phase boundaries for the

**SYS:** @@ same interactions resulted from the same POURBAIX Module

**SYS:** @@ calculation, are also plotted.

**SYS:** @@ -----

**SYS:** @@

**SYS:**

**SYS:**

**SYS:**

**SYS:** @@... Now, let's start using the advanced POURBAIX Module:

**SYS:** @@

**SYS:** go pour

... the command in full is GOTO\_MODULE

WELCOME TO THE POURBAIX MODULE  
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
for Quick Calculations of Pourbaix Diagrams  
=====

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 electropotential that is defined as Eh with the standard hydrogen electrode as the reference), but it is not defined as an aqueous species;
  - \* The vacancy (VA) is unnecessary for AQUEOUS solution phase and it should be avoided in the definition of phase-constituents in the AQUEOUS phase;
  - \* The AQUEOUS solution phase should always be defined as a constitutional solution phase, implying that all the aqueous solution species must be included in a single site, rather than in two or multiple sublattices.
- 4) Beside the AQUEOUS solution phase, there shall exist a GAS mixture phase containing at least H2O, 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, TCMF, SLAG, etc.) for Gaseous mixture phase and for various solid solution and stoichiometric compound phases. Furthermore, an experienced user can also utilize his/her own USER-specified databases in various cases.
- 6) The current advanced POURBAIX-Module has been designed and developed in an efficient and effective way that it only requires the user to just answer some simple and necessary questions, rather than to go through basic modules (i.e., TDB, GES5, POLY3 and POST) and type the ordinary command-lines. Beside the default plotted Pourbaix diagram, it also allows the user to easily and quickly plot many different properties of the system, stable phases and aqueous species, varied along the calculated phase boundaries for the same defined heterogeneous interaction system. Moreover, it permits the user to directly change some plotting settings and manipulate all kinds of plotted diagrams.
- 7) The current advanced POURBAIX-Module has been extended so that it is additionally able to directly perform a normal STEPPING calculation (varied with a specified independent variable) and to easily generate various types of property diagrams, for the same heterogeneous interaction system that has been defined in a previous POURBAIX or TDB-GES5-PLOY3-POST calculation.

-----

**Enforce a PAUSE after plotting when running a MACRO? /N/: ?**

Whenever running a Thermo-Calc MACRO (TCM) file, you may prefer to have a PAUSE after a specific diagram has been plotted on SCREEN, for the multiple purposes of efficiently and easily manipulating the plotted diagram directly on the traditional TC-Graph window or Java-based TC-UNITE window, such as:

- \* Printing it (of EMF/PS format) on connected printer(s);
- \* Converting it (of EMF format) to (PDF) graphical files;
- \* Saving it as an EMF graphical file;
- \* Dumping it as a PNG or BMP graphical file;
- \* Setting background colour for the current diagram and for all the sequential plots;
- \* Setting default font/size for all the sequential plots;
- \* Changing plotting Layers for all the sequential plots.

If no PAUSE is enforced, the POURBAIX Module will be going through all the sequential command-lines (answers) in the same POURBAIX session or till the SET\_INTERACTIVE\_MODE line in the MACRO file has been reached.

-----  
\*\* By Y(y), a PAUSE is always enforced after each diagram;  
\*\* By N(n), no PAUSE will be enforced at any point at all.  
-----  
Please then press <RETURN> at the PAUSE for continuation!

Enforce a PAUSE after plotting when running a MACRO? /N/: y

-----  
|  
| 1. Start a completely new POURBAIX diagram calculation |  
| 2. Open an old file & plot other property diagrams |  
| 3. Open an old file & make another POURBAIX calculation |  
| 4. Open an old file & make another STEPPING calculation |  
|  
|-----|

Select option /1/: ?

One of the four options (1/2/3/4) should be entered here:

- 1 -- Make a completely new POURBAIX diagram calculation and automatically plot a pH-Eh diagram.  
i.e., define a new chemical system;  
specify the T-P-X conditions;  
calculate the initial equilibria;  
perform the pH-Eh mapping calculation;  
plot pH-Eh & various property diagrams.
- 2 -- Open an existing POLY3 file created by POURBAIX Module (from a previous POURBAIX calculation Option 1 or 3 or a previous STEPPING calculation Option 4), and just selectively plot other property diagrams.  
i.e., open the old GES and POLY3 workspaces;  
plot pH-Eh or various property diagrams.
- 3 -- Open an existing POLY3 file created by POURBAIX Module and make another POURBAIX diagram calculation.  
i.e., open the old GES and POLY3 workspaces;  
adopt the defined chemical system;  
modify the T-P-X conditions;  
calculate the initial equilibria;  
perform the pH-Eh mapping calculation;  
plot pH-Eh & various property diagrams.
- 4 -- Open an existing POLY3 file created by POURBAIX Module (from a previous POURBAIX calculation Option 1 or 3 or a previous STEPPING calculation Option 4), and make a normal STEPPING calculation.  
i.e., open the old GES and POLY3 workspaces;  
adopt the defined chemical system;  
specify one of the T-P-X conditions as the stepping variable;  
calculate the initial equilibria;  
perform the stepping calculation;  
plot various property diagrams.

Select option /1/: 1

- 1 -- Make a completely new POURBAIX diagram calculation and automatically plot a pH-Eh diagram.  
i.e., define a new chemical system;  
specify the T-P-X conditions;  
calculate the initial equilibria;  
perform the pH-Eh mapping calculation;  
plot pH-Eh & various property diagrams.

Consider the GAS phase in calculating a Pourbaix diagram? /Y/: ?

You may optionally choose to ignore the GAS mixture phase on a calculated/plotted Pourbaix diagram. However, such a plot is actually not a complete Pourbaix diagram, due to that the thermodynamically-stable phase boundaries between the AQUEOUS solution phase and GAS mixture phase will not be calculated at all.

-----  
\*\* By Y(y), GAS mixture phase shall be always considered;  
\*\* By N(n), GAS mixture phase will be completely ignored.  
-----

Consider the GAS phase in calculating a Pourbaix diagram? /Y/: Y

Use single database? /Y/: Y

Combined Database: /PAQ2/: PAQ2

THERMODYNAMIC DATABASE module

Current database: Public Aqueous Soln (SIT) TDB v2.4

H	O	ZE
VA DEFINED		
LIQUID:L REJECTED		
GRAPHITE	DIAMOND_A4	FC_ORTHORHOMBIC
MONOCLINIC REJECTED		
CBCC_A12	CUB_A13	CHI_A12
FE4N	FECN_CHI REJECTED	
CEMENTITE	M23C6	M7C3
M5C2	M3C2	KSI_CARBIDE
PI REJECTED		
FE3C	NI3C	CR3C2
CR7C3	CR23C6 REJECTED	
COCO3	FECO3	NAHCO3
NA2CO3	NA2CO3_S2	NICO3
CR6O6 REJECTED		
CO3N	CRN	CR2N
FE2N	NI3N REJECTED	
NANO2	NANO2_S2	NANO3
REJECTED		
COCL2	CRCL2	CRCL3
FECL2	FECL3	NICL2
REJECTED		

FECLO                      NACLO4                      NACLO4\_S2  
REJECTED

DEFINE A CHEMICAL SYSTEM AND ITS INITIAL BULK COMPOSITION:

-----  
Normally a POURBAIX diagram and related equilibrium property in a heterogeneous interaction system are calculated under a certain bulk composition which is usually 1 kg of water with defined amounts of dissolving solute substances. The solutes may either be completely dissolved into the aqueous solution, or be partially dissolved and simultaneously form some solid phases.

CHEMICAL SYSTEM (ELEMENTS):  
Default defined elements (solvent H2O):        H & O  
and specially assigned ZE(electron) & VA(vacancy) .  
Prompt specified elements (solutes ELEM):  
Fe Ni Co Cr C N S Na Cl

INITIAL BULK COMPOSITION:  
Default defined composition (solvent):        1.0 kg of H2O  
Prompt specified composition (solutes):        x mole of ELEM  
-----

Notes: For accepting a default value, just RETURN at prompt;  
For changing to a specific value, enter it at prompt.

-----  
IMPORTANT NOTE for Entering Solutes in Chemical Formulas:  
First element letter in UPPER case, and second lower case!  
such as NaCl CO2 CoCl3 Fe0.93S NaSO4-1 H2SO4  
-----

Mass of Water (weight) = 1 kg

First solute: Fe  
Molality of Fe (mole/kg) /.001/: .001  
Second solute: NaCl .1  
Next solute:

-----  
Defined chemical system and initial bulk composition:  
Note: Solutes have been split up into chemical elements and their mole numbers. If confirmed, the POURBAIX Module will, in further steps, count the initial bulk composition in terms of chemical elements.  
-----

H2O	1.00000000	kg
ZE	(specially assigned)	
FE	0.1000000000E-02	mole
CL	0.1000000000E+00	mole
NA	0.1000000000E+00	mole

Confirm defined system and initial bulk composition? /Y/: Y

RETRIEVE THERMODYNAMIC DATA FROM THE DATABASE: PAQ2

H	O	ZE
VA DEFINED		
LIQUID:L REJECTED		
GRAPHITE	DIAMOND_A4	FC_ORTHORHOMBIC
MONOCLINIC REJECTED		
CBCC_A12	CUB_A13	CHI_A12
FE4N	FECN_CHI REJECTED	
CEMENTITE	M23C6	M7C3
M5C2	M3C2	KSI_CARBIDE
PI REJECTED		
FE3C	NI3C	CR3C2
CR7C3	CR23C6 REJECTED	
COCO3	FECO3	NAHCO3
NA2CO3	NA2CO3_S2	NICO3
CRC606 REJECTED		
CO3N	CRN	CR2N
FE2N	NI3N REJECTED	
NANO2	NANO2_S2	NANO3
REJECTED		
COCL2	CRCL2	CRCL3
FECL2	FECL3	NICL2
REJECTED		
FECLO	NACLO4	NACLO4_S2
REJECTED		
REINITIATING GES5 .....		
FE DEFINED		
CL DEFINED		
NA DEFINED		
/- DEFINED		

This database has following phases for the defined system

AQUEOUS:A	REF_ELECTRODE	GAS:G
FCC_A1	BCC_A2	HCP_A3
HALITE	WUSTITE	MAGNETITE
HEMATITE	FE2O3_GAMMA	FE02H2
FE03H3	FE0OH	FE2O2O2H2
NAO2	NA2O	NA2O_S2
NA2O_S3	NA2O2	NA2O2_S2
NAOH	NAOH_S2	NA2FE02

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	FE02H2	FE03H3
FE0OH	FE2O2O2H2	NAO2
NA2O	NA2O_S2	NA2O_S3
NA2O2	NA2O2_S2	NAOH
NAOH_S2	NA2FE02	

```

.....

OK? /Y/: Y
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

'TCS public data set for gaseous mixture in the Fe-Co-Cr-Na-Ni-C-H-O-N-S
-Cl system.'
'TCS public data set for liquid mixture and alloy solutions in the Fe-Co
-Cr-Na-Ni-C-H-O-N-S-Cl system.'
'TCS public data set for stoichiometric solids and liquids in the Fe-Co-Cr
-Na-Ni-C-H-O-N-S-Cl system.'
'TCS Aqueous Solution Database, TCAQ2, v2.0 (2002/2003). Extracted data
only for Fe-Co-Cr-Na-Ni-C-H-O-N-S-Cl bearing aqueous solution species
from TCAQ2 which covers totally 83 elements and contains many more
aqueous solution species.'
-OK-
Should any phase have a miscibility gap check? /N/: N

..... Reinitializing POLY3 workspaces .....

Enforce Global Minimization Technique in calculations? /N/: N

Save all functions, variables and tables in POLY3 file? /Y/: Y

Set numerical limits? /N/: N

SET CALCULATING PARAMETERS:

List of Default and Pre-defined Calculation Conditions:
-----
Units: T in K, P in Pascal, B(H2O) in gram, N(ELEM) in mole
-----
T=298.15, P=1E5, B(H2O)=1000, N(H+1)=0, N(ZE)=0, N(CL)=0.1, N(FE)=1E-3,
N(NA)=0.1
DEGREES OF FREEDOM 0

Confirm defined conditions? /Y/: Y

Calculating start points; please be patient!

LIST THE FIRST DEFAULT STARTING EQUILIBRIUM POINT:

Output from POLY-3, equilibrium = 1, label A0 , database: PAQ2

Conditions:
T=298.15, P=1E5, B(H2O)=1000, N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.1181, MUR(ZE)=100
DEGREES OF FREEDOM 0

Temperature 298.15 K ( 25.00 C), Pressure 1.000000E+05
Number of moles of components 5.57094E+01, Mass in grams 1.00590E+03
Total Gibbs energy -1.70696E+07, Enthalpy -1.59069E+07, Volume 0.00000E+00

Component      Moles      M-Fraction  Activity  Potential  Ref.stat
CL              1.0000E-01  1.7950E-03  1.4499E-30 -1.7032E+05 SER
FE              1.0000E-03  1.7950E-05  4.6321E-26 -1.4461E+05 SER
H+1             -3.0000E-03 -5.3851E-05  1.0000E-07 -3.9956E+04 SER
NA              1.0000E-01  1.7950E-03  1.7205E-50 -2.8406E+05 SER
H2O             5.5508E+01  9.9639E-01  9.9593E-01 -1.0110E+01 AQUEOUS
ZE              3.0000E-03  5.3851E-05  1.0412E+00  1.0000E+02 REF_ELEC

AQUEOUS
Status ENTERED      Driving force 0.0000E+00
Moles 5.5707E+01, Mass 1.0058E+03, Volume fraction 0.0000E+00 Mole fractions:
H2O 9.96410E-01 NA 1.79511E-03 FE 1.08146E-11
CL 1.79511E-03 ZE 2.03381E-11 H+1 -1.36468E-11
Constitution:
SiteFraction      Molality      Activity      log10Act
H2O 9.96410E-01 5.55084E+01 9.96012E-01 -0.0017
CL-1 1.79511E-03 1.00003E-01 7.76756E-02 -1.1097
NA+1 1.79511E-03 1.00003E-01 7.76756E-02 -1.1097
OH-1 2.31689E-09 1.29070E-07 1.00218E-07 -6.9991
H+1 2.30788E-09 1.28568E-07 1.00000E-07 -7.0000
FE+2 6.21477E-12 3.46215E-10 1.26203E-10 -9.8989
FEOH+1 4.59380E-12 2.55913E-10 1.99003E-10 -9.7011
O3 1.00000E-15 0.00000E+00 2.6033E-113 -112.5845
H2O2 1.00000E-15 0.00000E+00 3.63324E-46 -45.4397
HClO 1.00000E-15 0.00000E+00 3.55905E-45 -44.4487
H2 1.00000E-15 0.00000E+00 5.46000E-18 -17.2628
HClO2 1.00000E-15 0.00000E+00 1.38939E-87 -86.8572
FEOH+2 1.00000E-15 0.00000E+00 9.27035E-19 -18.0329
HO2-1 1.00000E-15 0.00000E+00 7.68880E-51 -50.1141
FeO3H3-1 1.00000E-15 0.00000E+00 1.69673E-51 -50.7704
FeCL+2 1.00000E-15 0.00000E+00 3.39801E-23 -22.4688
Fe2O2H2+4 1.00000E-15 0.00000E+00 3.71405E-35 -34.4302
FE+3 1.00000E-15 0.00000E+00 1.53892E-23 -22.8128
O2 1.00000E-15 0.00000E+00 2.54948E-58 -57.5935
ClO4-1 1.00000E-15 0.00000E+00 8.8489E-133 -132.0531
ClO3-1 1.00000E-15 0.00000E+00 1.5694E-105 -104.8043
ClO2-1 1.00000E-15 0.00000E+00 1.45414E-82 -81.8374
ClO2 1.00000E-15 0.00000E+00 1.6417E-100 -99.7847
ClO-1 1.00000E-15 0.00000E+00 7.71560E-46 -45.1126
CL2 1.00000E-15 0.00000E+00 5.82418E-50 -49.2348
Solution Properties: pH = 7.0000 Eh = 0.0010 V I = 0.1000
pe = 0.0175 Ah = 0.1000 kJ m° = 0.2000
Aw = 0.9960 Os = 1.1089 pKw = 13.9973
At1= 1.0000E-15 At2= 1.2907E-07 (equiv_mol/kg_H2O)

HEMATITE
Status ENTERED      Driving force 0.0000E+00
Moles 2.5000E-03, Mass 7.9846E-02, Volume fraction 0.0000E+00 Mole fractions:
ZE 1.20000E+00 FE 4.00000E-01 NA 0.00000E+00
H2O 6.00000E-01 CL 0.00000E+00 H+1 -1.20000E+00
Constitution:

```

FE2O3 1.00000E+00

LIST THE DEFINED SYMBOLS:

DEFINED CONSTANTS

TSLIMIT0=99, AH2O=55.508435, WH2O=1.80152E-2, RNL=2.3025851, R=8.31451,  
RNF=96485.309

DEFINED FUNCTIONS AND VARIABLES%

TC%=T-273.15  
PBAR%=P\*1E-05  
PKB%=P\*1E-08  
RT%=R\*T  
EH=MUR(ZE)/RNF  
PH=- LOG10 (ACR (H+1,AQUEOUS) \*AH2O )  
YH2O=Y (AQUEOUS,H2O)  
ACRH2O=ACR (H2O,AQUEOUS)  
RCH2O=ACR (H2O,AQUEOUS)  
MLH2O=AH2O  
ACTW=ACRH2O  
OSMC=-YH2O/ (1-YH2O ) \* LOG (ACRH2O )  
TMI= (1-YH2O ) \*AH2O/YH2O  
AHZE=MUR (ZE) /1000  
PEZE=MUR (ZE) / (RNL\*RT )  
AI1=ACR (CL-1,AQUEOUS) \*AH2O  
RC1=ACR (CL-1,AQUEOUS) \*YH2O/Y (AQUEOUS,CL-1)  
ML1=Y (AQUEOUS,CL-1) \*AH2O/YH2O  
AI2=ACR (CL2,AQUEOUS) \*AH2O  
RC2=ACR (CL2,AQUEOUS) \*YH2O/Y (AQUEOUS,CL2)  
ML2=Y (AQUEOUS,CL2) \*AH2O/YH2O  
AI3=ACR (CLO-1,AQUEOUS) \*AH2O  
RC3=ACR (CLO-1,AQUEOUS) \*YH2O/Y (AQUEOUS,CLO-1)  
ML3=Y (AQUEOUS,CLO-1) \*AH2O/YH2O  
AI4=ACR (CLO2,AQUEOUS) \*AH2O  
RC4=ACR (CLO2,AQUEOUS) \*YH2O/Y (AQUEOUS,CLO2)  
ML4=Y (AQUEOUS,CLO2) \*AH2O/YH2O  
AI5=ACR (CLO2-1,AQUEOUS) \*AH2O  
RC5=ACR (CLO2-1,AQUEOUS) \*YH2O/Y (AQUEOUS,CLO2-1)  
ML5=Y (AQUEOUS,CLO2-1) \*AH2O/YH2O  
AI6=ACR (CLO3-1,AQUEOUS) \*AH2O  
RC6=ACR (CLO3-1,AQUEOUS) \*YH2O/Y (AQUEOUS,CLO3-1)  
ML6=Y (AQUEOUS,CLO3-1) \*AH2O/YH2O  
AI7=ACR (CLO4-1,AQUEOUS) \*AH2O  
RC7=ACR (CLO4-1,AQUEOUS) \*YH2O/Y (AQUEOUS,CLO4-1)  
ML7=Y (AQUEOUS,CLO4-1) \*AH2O/YH2O  
AI8=ACR (FE+2,AQUEOUS) \*AH2O  
RC8=ACR (FE+2,AQUEOUS) \*YH2O/Y (AQUEOUS,FE+2)  
ML8=Y (AQUEOUS,FE+2) \*AH2O/YH2O  
AI9=ACR (FE+3,AQUEOUS) \*AH2O  
RC9=ACR (FE+3,AQUEOUS) \*YH2O/Y (AQUEOUS,FE+3)  
ML9=Y (AQUEOUS,FE+3) \*AH2O/YH2O  
AI10=ACR (FE2O2H2+4,AQUEOUS) \*AH2O  
RC10=ACR (FE2O2H2+4,AQUEOUS) \*YH2O/Y (AQUEOUS,FE2O2H2+4)  
ML10=Y (AQUEOUS,FE2O2H2+4) \*AH2O/YH2O  
AI11=ACR (FECL+2,AQUEOUS) \*AH2O  
RC11=ACR (FECL+2,AQUEOUS) \*YH2O/Y (AQUEOUS,FECL+2)  
ML11=Y (AQUEOUS,FECL+2) \*AH2O/YH2O  
AI12=ACR (FEO3H3-1,AQUEOUS) \*AH2O  
RC12=ACR (FEO3H3-1,AQUEOUS) \*YH2O/Y (AQUEOUS,FEO3H3-1)  
ML12=Y (AQUEOUS,FEO3H3-1) \*AH2O/YH2O  
AI13=ACR (FEOH+1,AQUEOUS) \*AH2O  
RC13=ACR (FEOH+1,AQUEOUS) \*YH2O/Y (AQUEOUS,FEOH+1)  
ML13=Y (AQUEOUS,FEOH+1) \*AH2O/YH2O  
AI14=ACR (FEOH+2,AQUEOUS) \*AH2O  
RC14=ACR (FEOH+2,AQUEOUS) \*YH2O/Y (AQUEOUS,FEOH+2)  
ML14=Y (AQUEOUS,FEOH+2) \*AH2O/YH2O  
AI15=ACR (H+1,AQUEOUS) \*AH2O  
RC15=ACR (H+1,AQUEOUS) \*YH2O/Y (AQUEOUS,H+1)  
ML15=Y (AQUEOUS,H+1) \*AH2O/YH2O  
AI16=ACR (H2,AQUEOUS) \*AH2O  
RC16=ACR (H2,AQUEOUS) \*YH2O/Y (AQUEOUS,H2)  
ML16=Y (AQUEOUS,H2) \*AH2O/YH2O  
AI17=ACR (H2O,AQUEOUS)  
RC17=ACR (H2O,AQUEOUS) /Y (AQUEOUS,H2O)  
ML17=Y (AQUEOUS,H2O) \*AH2O/YH2O  
AI18=ACR (H2O2,AQUEOUS) \*AH2O  
RC18=ACR (H2O2,AQUEOUS) \*YH2O/Y (AQUEOUS,H2O2)  
ML18=Y (AQUEOUS,H2O2) \*AH2O/YH2O  
AI19=ACR (HCLO,AQUEOUS) \*AH2O  
RC19=ACR (HCLO,AQUEOUS) \*YH2O/Y (AQUEOUS,HCLO)  
ML19=Y (AQUEOUS,HCLO) \*AH2O/YH2O  
AI20=ACR (HCLO2,AQUEOUS) \*AH2O  
RC20=ACR (HCLO2,AQUEOUS) \*YH2O/Y (AQUEOUS,HCLO2)  
ML20=Y (AQUEOUS,HCLO2) \*AH2O/YH2O  
AI21=ACR (HO2-1,AQUEOUS) \*AH2O  
RC21=ACR (HO2-1,AQUEOUS) \*YH2O/Y (AQUEOUS,HO2-1)  
ML21=Y (AQUEOUS,HO2-1) \*AH2O/YH2O  
AI22=ACR (NA+1,AQUEOUS) \*AH2O  
RC22=ACR (NA+1,AQUEOUS) \*YH2O/Y (AQUEOUS,NA+1)  
ML22=Y (AQUEOUS,NA+1) \*AH2O/YH2O  
AI23=ACR (O2,AQUEOUS) \*AH2O  
RC23=ACR (O2,AQUEOUS) \*YH2O/Y (AQUEOUS,O2)  
ML23=Y (AQUEOUS,O2) \*AH2O/YH2O  
AI24=ACR (O3,AQUEOUS) \*AH2O  
RC24=ACR (O3,AQUEOUS) \*YH2O/Y (AQUEOUS,O3)  
ML24=Y (AQUEOUS,O3) \*AH2O/YH2O  
AI25=ACR (OH-1,AQUEOUS) \*AH2O  
RC25=ACR (OH-1,AQUEOUS) \*YH2O/Y (AQUEOUS,OH-1)  
ML25=Y (AQUEOUS,OH-1) \*AH2O/YH2O  
IS1=.5\*ML1+.5\*ML3+.5\*ML5  
IS2=.5\*ML6+.5\*ML7+.5\*ML8\*2\*\*2  
IS3=.5\*ML9\*3\*\*2+.5\*ML10\*4\*\*2+.5\*ML11\*2\*\*2  
IS4=.5\*ML12+.5\*ML13+.5\*ML14\*2\*\*2  
IS5=.5\*ML15+.5\*ML21+.5\*ML22  
ISTR=1\*IS1+1\*IS2+1\*IS3+1\*IS4+1\*IS5  
RLOGH= LOG10 (ACR (H+1,AQUEOUS) \*AH2O )  
RLOGOH= LOG10 (ACR (OH-1,AQUEOUS) \*AH2O )  
RLOGH2O= LOG10 (ACRH2O )

DEFINED TABLES

GPT=T, P, PH, EH, ISTR  
SFT=Y (AQUEOUS,CL-1), Y (AQUEOUS,CL2), Y (AQUEOUS,CLO-1), Y (AQUEOUS,CLO2),  
Y (AQUEOUS,CLO2-1), Y (AQUEOUS,CLO3-1), Y (AQUEOUS,CLO4-1),  
Y (AQUEOUS,FE+2), Y (AQUEOUS,FE+3), Y (AQUEOUS,FE2O2H2+4),  
Y (AQUEOUS,FECL+2), Y (AQUEOUS,FEO3H3-1), Y (AQUEOUS,FEOH+1),  
Y (AQUEOUS,FEOH+2), Y (AQUEOUS,H+1), Y (AQUEOUS,H2), Y (AQUEOUS,H2O),  
Y (AQUEOUS,H2O2), Y (AQUEOUS,HCLO), Y (AQUEOUS,HCLO2), Y (AQUEOUS,HO2-1),  
Y (AQUEOUS,NA+1), Y (AQUEOUS,O2), Y (AQUEOUS,O3), Y (AQUEOUS,OH-1), PH, EH  
AYT=AC (CL-1,AQUEOUS), AC (CL2,AQUEOUS), AC (CLO-1,AQUEOUS),

```

AC(CLO2,AQUEOUS), AC(CLO2-1,AQUEOUS), AC(CLO3-1,AQUEOUS),
AC(CLO4-1,AQUEOUS), AC(Fe+2,AQUEOUS), AC(Fe+3,AQUEOUS),
AC(Fe2O2H2+4,AQUEOUS), AC(FeCL+2,AQUEOUS), AC(FeO3H3-1,AQUEOUS),
AC(FeOH+1,AQUEOUS), AC(FeOH+2,AQUEOUS), AC(H+1,AQUEOUS),
AC(H2,AQUEOUS), AC(H2O,AQUEOUS), AC(H2O2,AQUEOUS), AC(HCLO,AQUEOUS),
AC(HCLO2,AQUEOUS), AC(HO2-1,AQUEOUS), AC(NA+1,AQUEOUS), AC(O2,AQUEOUS),
AC(O3,AQUEOUS), AC(OH-1,AQUEOUS), PH, EH
ART=ACR(CL-1,AQUEOUS), ACR(CL2,AQUEOUS), ACR(CLO-1,AQUEOUS),
ACR(CLO2,AQUEOUS), ACR(CLO2-1,AQUEOUS), ACR(CLO3-1,AQUEOUS),
ACR(CLO4-1,AQUEOUS), ACR(Fe+2,AQUEOUS), ACR(Fe+3,AQUEOUS),
ACR(Fe2O2H2+4,AQUEOUS), ACR(FeCL+2,AQUEOUS), ACR(FeO3H3-1,AQUEOUS),
ACR(FeOH+1,AQUEOUS), ACR(FeOH+2,AQUEOUS), ACR(H+1,AQUEOUS),
ACR(H2,AQUEOUS), ACR(H2O,AQUEOUS), ACR(H2O2,AQUEOUS),
ACR(HCLO,AQUEOUS), ACR(HCLO2,AQUEOUS), ACR(HO2-1,AQUEOUS),
ACR(NA+1,AQUEOUS), ACR(O2,AQUEOUS), ACR(O3,AQUEOUS), ACR(OH-1,AQUEOUS),
PH, EH
AIT=AI1, AI2, AI3, AI4, AI5, AI6, AI7, AI8, AI9, AI10, AI11, AI12, AI13,
AI14, AI15, AI16, AI17, AI18, AI19, AI20, AI21, AI22, AI23, AI24, AI25,
PH, EH
RCT=RC1, RC2, RC3, RC4, RC5, RC6, RC7, RC8, RC9, RC10, RC11, RC12, RC13,
RC14, RC15, RC16, RC17, RC18, RC19, RC20, RC21, RC22, RC23, RC24, RC25,
PH, EH
MLT=ML1, ML2, ML3, ML4, ML5, ML6, ML7, ML8, ML9, ML10, ML11, ML12, ML13,
ML14, ML15, ML16, ML18, ML19, ML20, ML21, ML22, ML23, ML24, ML25, ISTR,
PH, EH

```

#### IMPORTANT FACTS:

The default definitions of the Eh and pH quantities in the advanced POURBAIX-Module (and in the ordinary TDB-GES-POLY calculation routines) should ALWAYS be as below:

```

Eh = MUR(ZE)/RNF
pH = -log10[AI(H+1,AQUEOUS)]
    = -log10[ACR(H+1,AQUEOUS)*AH2O]
where RNF is the Faraday constant (96485.309 C/mol),
and AH2O is the molecular weight of H2O (55.508435 g).
MUR(ZE) is the electrochemical potential (ECP; in the
unit of J/mol; w.r.t. the standard hydrogen electrode).
ACR(H+1,AQUEOUS) is the site-fraction-based activity of
the H+1 aqueous species in AQUEOUS solution phase, but
AI(H+1,AQUEOUS) [that equals ACR(H+1,AQUEOUS)*AH2O] is
the molality-based activity of the H+1 aqueous species
that should be used for defining the pH quantity.

```

Within an aqueous-bearing heterogeneous interaction system, the fundamental system-components must be H2O, H+1 and ZE, which are corresponding to the basic elements O & H and the hypothetical electron (ZE) in the aqueous solution phase. For the additional chemical elements in the system, their corresponding system-components shall be defined as in their element forms (such as Fe, Cr, Mn, Ni, Na, Cl, S) or (for some) in their molecular forms (e.g., NaCl, H2S). The reference state for the H2O component must always be defined as the solvent species H2O in the AQUEOUS solution phase under the current temperature (\*) and 100000 Pascal (i.e., 1 bar). The reference states for the H+1 and ZE components are by default set as their SER.

Various conventional properties of aqueous solute species I are converted in the following manners:

```

ML = Y(AQUEOUS,I)*AH2O/YH2O
RC = ACR(I,AQUEOUS)*YH2O/Y(AQUEOUS,I)
AI = RC*ML
    = ACR(I,AQUEOUS)*AH2O
where YH2O [i.e., Y(AQUEOUS,H2O)] and Y(AQUEOUS,I) are
the site-fractions of solvent H2O and solute species I.

```

#### LIST THE DEFINED AXIS-VARIABLES:

```

Axis No 1: LNACR(H+1)           Min: -34.532608Max: 2.3025851 Inc: 0.8
Axis No 2: MUR(ZE)              Min: -150000   Max: 200000   Inc: 7718.85

```

NOTE: The default settings (listed above) for two mapping variables [in terms of lnACR(H+1) and MUR(ZE), and their minimum/maximum values and increment steps] are covering the following pH-Eh ranges/steps:

```

pH:  0.00 -> 14.00, at a step of 0.35
Eh: -1.55 ->  2.07, at a step of 0.08 (V)

```

The maximum pH limit has been calculated precisely and determined automatically by the POURBAIX-Module, as a function of the temperature-pressure conditions and initial bulk compositions of the current defined interaction system.

Accept the default settings for two mapping variables? /Y/: Y

#### LIST ALL THE INITIAL EQUILIBRIA FOR MAPPING:

```

No 1  +2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(Fe)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=100.
No 2  -2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(Fe)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=100.
No 3  +1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(Fe)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=100.
No 4  -1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(Fe)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=100.
No 5  +2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(Fe)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=-28400
No 6  -2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(Fe)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=-28400
No 7  +1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(Fe)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=-28400
No 8  -1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(Fe)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=-28400
No 9  +2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(Fe)=1E-3, N(NA)=0.1,
LNACR(H+1)=-9.2103404, MUR(ZE)=-13000
No 10 -2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(Fe)=1E-3, N(NA)=0.1,
LNACR(H+1)=-9.2103404, MUR(ZE)=-13000
No 11 +1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(Fe)=1E-3, N(NA)=0.1,
LNACR(H+1)=-9.2103404, MUR(ZE)=-13000
No 12 -1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(Fe)=1E-3, N(NA)=0.1,
LNACR(H+1)=-9.2103404, MUR(ZE)=-13000
No 13 +2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(Fe)=1E-3, N(NA)=0.1,
LNACR(H+1)=-9.2103404, MUR(ZE)=86837
No 14 -2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(Fe)=1E-3, N(NA)=0.1,

```

```

LNACR(H+1)=-9.2103404, MUR(ZE)=86837
No 15 +1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-9.2103404, MUR(ZE)=86837
No 16 -1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-9.2103404, MUR(ZE)=86837
No 17 +2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=66000.
No 18 -2> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=66000.
No 19 +1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=66000.
No 20 -1> T=298.15, P=100000, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1,
LNACR(H+1)=-16.118096, MUR(ZE)=66000.

```

MAP THE POURBAIX DIAGRAM:  
Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Tie-lines not in the plane of calculation

```

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28
Generating start point 29
Generating start point 30
Working hard
Generating start point 31
Generating start point 32
Generating start point 33
Generating start point 34
Generating start point 35
Generating start point 36
Generating start point 37
Generating start point 38
Generating start point 39
Generating start point 40
Working hard
Generating start point 41
Generating start point 42
Generating start point 43
Generating start point 44
Generating start point 45
Generating start point 46

```

```

Phase region boundary 1 at: -1.612E+01 7.911E+04
GAS
AQUEOUS
** HALITE
HEMATITE
Calculated.. 25 equilibria
Terminating at axis limit.

```

```

Phase region boundary 2 at: -3.453E+01 3.383E+04
GAS
AQUEOUS
** HALITE
HEMATITE
Calculated. 42 equilibria

```

```

Phase region boundary 3 at: -2.296E+00 1.134E+05
GAS
AQUEOUS
** HALITE
** HEMATITE

```

```

Phase region boundary 4 at: -2.296E+00 1.134E+05
GAS
AQUEOUS
** HALITE
Calculated 33 equilibria

```

```

Phase region boundary 5 at: -2.296E+00 1.134E+05
GAS
AQUEOUS
** HEMATITE
Calculated 5 equilibria

```

```

Phase region boundary 6 at: -2.296E+00 1.134E+05
GAS
AQUEOUS
HALITE
** HEMATITE
Calculated 31 equilibria

```

```

Phase region boundary 7 at: -1.612E+01 7.911E+04
GAS

```



```

    AQUEOUS
** HALITE
    HEMATITE
Calculated.          19 equilibria
Terminating at known equilibrium

Phase region boundary  8 at: -1.612E+01  7.817E+04
** GAS
    AQUEOUS
    HEMATITE
Calculated..         26 equilibria
Terminating at axis limit.

Phase region boundary  9 at: -3.453E+01  3.296E+04
** GAS
    AQUEOUS
    HEMATITE
Calculated.          43 equilibria

Phase region boundary 10 at: -1.975E+00  1.132E+05
** GAS
    AQUEOUS
** HEMATITE

Phase region boundary 11 at: -1.975E+00  1.132E+05
** GAS
    AQUEOUS
Calculated..         9 equilibria
Terminating at axis limit.

Phase region boundary 12 at: -1.975E+00  1.132E+05
    AQUEOUS
** HEMATITE
Calculated.          30 equilibria

Phase region boundary 13 at: -1.420E+01 -2.225E+04
    AQUEOUS
** HEMATITE
** MAGNETITE

Phase region boundary 14 at: -1.420E+01 -2.225E+04
    AQUEOUS
** HEMATITE
    MAGNETITE
Calculated..         30 equilibria
Terminating at axis limit.

Phase region boundary 15 at: -1.420E+01 -2.225E+04
    AQUEOUS
** MAGNETITE
Calculated.          4 equilibria

Phase region boundary 16 at: -1.625E+01 -4.067E+04
** GAS
    AQUEOUS
** MAGNETITE

Phase region boundary 17 at: -1.625E+01 -4.067E+04
    GAS
    AQUEOUS
** MAGNETITE
Calculated           34 equilibria

Phase region boundary 18 at: -1.625E+01 -4.067E+04
** GAS
    AQUEOUS
Calculated..         28 equilibria
Terminating at axis limit.

Phase region boundary 19 at: -1.625E+01 -4.067E+04
** GAS
    AQUEOUS
    MAGNETITE
Calculated..         27 equilibria
Terminating at axis limit.

Phase region boundary 20 at: -1.420E+01 -2.225E+04
    AQUEOUS
    HEMATITE
** MAGNETITE
Calculated..         30 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 21 at: -1.975E+00  1.132E+05
    GAS
    AQUEOUS
** HEMATITE
Calculated           11 equilibria

Phase region boundary 22 at: -1.612E+01  7.817E+04
** GAS
    AQUEOUS
    HEMATITE
Calculated.          19 equilibria
Terminating at known equilibrium

Phase region boundary 23 at: -1.612E+01 -2.701E+04
    AQUEOUS
    HEMATITE
** MAGNETITE
Calculated..         26 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 24 at: -1.612E+01 -2.701E+04
    AQUEOUS
    HEMATITE
** MAGNETITE
Calculated.          4 equilibria
Terminating at known equilibrium

Phase region boundary 25 at: -1.116E+01  1.000E+02
    AQUEOUS
** HEMATITE
Calculated.          7 equilibria

```

Terminating at known equilibrium

Phase region boundary 26 at: -1.116E+01 1.000E+02  
 AQUEOUS  
 \*\* HEMATITE  
 Calculated. 24 equilibria  
 Terminating at known equilibrium

Phase region boundary 27 at: -1.612E+01 -2.701E+04  
 AQUEOUS  
 \*\* HEMATITE  
 MAGNETITE  
 Calculated.. 26 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 28 at: -1.612E+01 -2.701E+04  
 AQUEOUS  
 \*\* HEMATITE  
 MAGNETITE  
 Calculated. 4 equilibria  
 Terminating at known equilibrium

Phase region boundary 29 at: -1.612E+01 -3.959E+04  
 AQUEOUS  
 \*\* MAGNETITE  
 Calculated. 2 equilibria  
 Terminating at known equilibrium

Phase region boundary 30 at: -1.612E+01 -3.959E+04  
 AQUEOUS  
 \*\* MAGNETITE  
 Calculated. 4 equilibria  
 Terminating at known equilibrium

Phase region boundary 31 at: -1.485E+01 -2.840E+04  
 AQUEOUS  
 \*\* MAGNETITE  
 Calculated. 3 equilibria  
 Terminating at known equilibrium

Phase region boundary 32 at: -1.485E+01 -2.840E+04  
 AQUEOUS  
 \*\* MAGNETITE  
 Calculated. 2 equilibria  
 Terminating at known equilibrium

Phase region boundary 33 at: -1.668E+01 -2.840E+04  
 AQUEOUS  
 \*\* HEMATITE  
 MAGNETITE  
 Calculated.. 26 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 34 at: -1.668E+01 -2.840E+04  
 AQUEOUS  
 \*\* HEMATITE  
 MAGNETITE  
 Calculated. 5 equilibria  
 Terminating at known equilibrium

Phase region boundary 35 at: -9.172E+00 9.539E+04  
 \*\* GAS  
 AQUEOUS  
 HEMATITE  
 Calculated.. 35 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 36 at: -9.172E+00 9.539E+04  
 \*\* GAS  
 AQUEOUS  
 HEMATITE  
 Calculated. 11 equilibria  
 Terminating at known equilibrium

Phase region boundary 37 at: -9.210E+00 9.529E+04  
 \*\* GAS  
 AQUEOUS  
 HEMATITE  
 Calculated.. 35 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 38 at: -9.210E+00 9.529E+04  
 \*\* GAS  
 AQUEOUS  
 HEMATITE  
 Calculated. 11 equilibria  
 Terminating at known equilibrium

Phase region boundary 39 at: -9.210E+00 1.461E+04  
 AQUEOUS  
 \*\* HEMATITE  
 Calculated. 8 equilibria  
 Terminating at known equilibrium

Phase region boundary 40 at: -9.210E+00 1.461E+04  
 AQUEOUS  
 \*\* HEMATITE  
 Calculated. 25 equilibria  
 Terminating at known equilibrium

Phase region boundary 41 at: -9.210E+00 -2.323E+04  
 \*\* GAS  
 AQUEOUS  
 Calculated. 10 equilibria  
 Terminating at known equilibrium

Phase region boundary 42 at: -9.210E+00 -2.323E+04  
 \*\* GAS  
 AQUEOUS  
 Calculated.. 18 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 43 at: -5.086E+00 -1.300E+04  
 \*\* GAS  
 AQUEOUS  
 Calculated. 16 equilibria  
 Terminating at known equilibrium

Phase region boundary 44 at: -5.086E+00 -1.300E+04  
 \*\* GAS  
 AQUEOUS  
 Calculated.. 13 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 45 at: -1.293E+01 -1.300E+04  
 AQUEOUS  
 \*\* HEMATITE  
 Calculated. 3 equilibria  
 Terminating at known equilibrium

Phase region boundary 46 at: -1.293E+01 -1.300E+04  
 AQUEOUS  
 \*\* HEMATITE  
 Calculated. 27 equilibria  
 Terminating at known equilibrium

Phase region boundary 47 at: -9.210E+00 9.529E+04  
 \*\* GAS  
 AQUEOUS  
 HEMATITE  
 Calculated.. 35 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 48 at: -9.210E+00 9.529E+04  
 \*\* GAS  
 AQUEOUS  
 HEMATITE  
 Calculated. 11 equilibria  
 Terminating at known equilibrium

Phase region boundary 49 at: -9.210E+00 -2.323E+04  
 \*\* GAS  
 AQUEOUS  
 Calculated. 10 equilibria  
 Terminating at known equilibrium

Phase region boundary 50 at: -9.210E+00 -2.323E+04  
 \*\* GAS  
 AQUEOUS  
 Calculated.. 18 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 51 at: -9.210E+00 1.461E+04  
 AQUEOUS  
 \*\* HEMATITE  
 Calculated. 8 equilibria  
 Terminating at known equilibrium

Phase region boundary 52 at: -9.210E+00 1.461E+04  
 AQUEOUS  
 \*\* HEMATITE  
 Calculated. 25 equilibria  
 Terminating at known equilibrium

Phase region boundary 53 at: -1.975E+00 8.684E+04  
 AQUEOUS  
 \*\* HEMATITE  
 Calculated. 26 equilibria  
 Terminating at known equilibrium

Phase region boundary 54 at: -1.975E+00 8.684E+04  
 AQUEOUS  
 \*\* HEMATITE  
 Calculated. 5 equilibria  
 Terminating at known equilibrium

Phase region boundary 55 at: -1.262E+01 8.684E+04  
 \*\* GAS  
 AQUEOUS  
 HEMATITE  
 Calculated.. 31 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 56 at: -1.262E+01 8.684E+04  
 \*\* GAS  
 AQUEOUS  
 HEMATITE  
 Calculated. 15 equilibria  
 Terminating at known equilibrium

Phase region boundary 57 at: -1.612E+01 7.817E+04  
 \*\* GAS  
 AQUEOUS  
 HEMATITE  
 Calculated.. 26 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 58 at: -1.612E+01 7.817E+04  
 \*\* GAS  
 AQUEOUS  
 HEMATITE  
 Calculated. 19 equilibria  
 Terminating at known equilibrium

Phase region boundary 59 at: -1.612E+01 -2.701E+04  
 AQUEOUS  
 HEMATITE  
 \*\* MAGNETITE  
 Calculated.. 26 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 60 at: -1.612E+01 -2.701E+04  
 AQUEOUS  
 HEMATITE  
 \*\* MAGNETITE  
 Calculated. 4 equilibria  
 Terminating at known equilibrium

Phase region boundary 61 at: -2.438E+00 6.600E+04  
 AQUEOUS  
 \*\* HEMATITE  
 Calculated. 24 equilibria  
 Terminating at known equilibrium

Phase region boundary 62 at: -2.438E+00 6.600E+04  
 AQUEOUS  
 \*\* HEMATITE  
 Calculated. 9 equilibria  
 Terminating at known equilibrium

Phase region boundary 63 at: -2.103E+01 6.600E+04  
 \*\* GAS  
 AQUEOUS  
 HEMATITE  
 Calculated.. 20 equilibria  
 Terminating at known equilibrium  
 Terminating at axis limit.

Phase region boundary 64 at: -2.103E+01 6.600E+04  
 \*\* GAS  
 AQUEOUS  
 HEMATITE  
 Calculated. 26 equilibria  
 Terminating at known equilibrium  
 \*\*\* BUFFER SAVED ON FILE:  
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex40\POUR  
 BAIX.POLY3  
 CPU time for mapping 225 seconds

POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

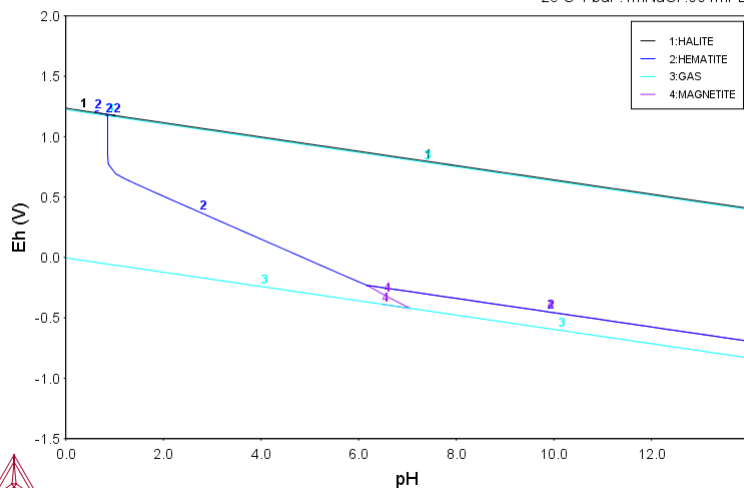
CURRENT DEVICE: TC-UNITE Driver

Plotting the diagram; please be patient!

### Pourbaix Diagram

2016.05.17.21.33.19  
 CL, FE, H+1, NA, H2O, ZE  
 T=298.15, P=1E5, B(H2O)=1000, N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1

25 C 1 bar .1mNaCl .001mFE



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

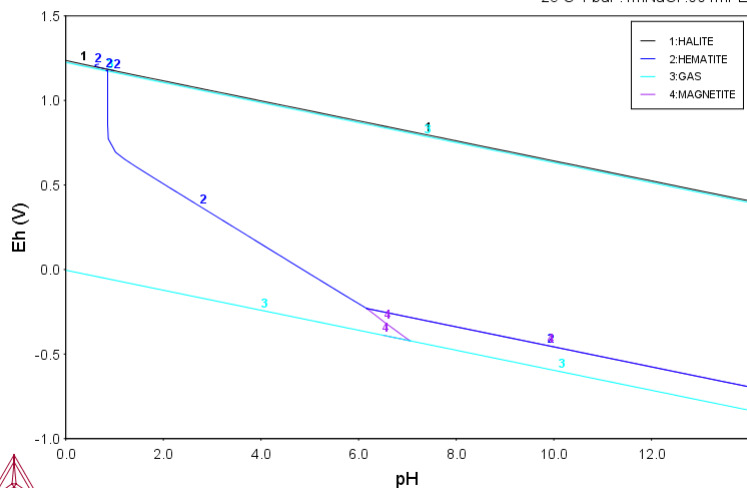
CURRENT DEVICE: TC-UNITE Driver

Plotting the diagram; please be patient!

# Pourbaix Diagram

2016.05.17.21.33.19  
CL, FE, H+1, NA, H2O, ZE  
T=298.15, P=1E5, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1

25 C 1 bar .1mNaCl .001mFE



Hit RETURN to continue

Another zoom? /N/: N

Change Curve-Label Option for the diagram? /N/: N

Add Label-Texts onto the Pourbaix diagram? /N/: N

Change the Subtitle of the diagram? /N/: N

Change Axis-Texts? /N/: N

Further Refine the diagram in POST Module? /N/: N

Hard copy of the diagram? /N/: n

Save X-Y coordinates of curve on text file? /N/: y

File name /POURBAIX/: TCEX40-1.EXP

Modify the diagram? /N/: y

Zoom in? /N/: N

Change Curve-Label Option for the diagram? /N/: N

Add Label-Texts onto the Pourbaix diagram? /N/: y

At what pH-Eh point add the label text?

X-pH /1.2/: 1.2

Y-Eh /.25/: 0.25

Automatic phase labels? /N/: N

Text? /Aqs/: Aqs

Text size: /.36/: 0.26

Another Label Text to be added? /N/: y

At what pH-Eh point add the label text?

X-pH /2.599732093/: 8

Y-Eh /.5/: 0.25

Automatic phase labels? /N/: N

Text? /Aqs/: Aqs+Hm

Text size: /.36/: 0.26

Another Label Text to be added? /N/: y

At what pH-Eh point add the label text?

X-pH /9.399732093/: 8

Y-Eh /.5/: -0.3

Automatic phase labels? /N/: N

Text? /Aqs/: Aqs+Mt

Text size: /.36/: 0.26

Another Label Text to be added? /N/: y

At what pH-Eh point add the label text?

X-pH /9.399732093/: 8

Y-Eh /-.05/: 1.1

Automatic phase labels? /N/: N

Text? /Aqs/: Gas (O2-dominant)

Text size: /.36/: 0.26

Another Label Text to be added? /N/: y

At what pH-Eh point add the label text?

X-pH /9.399732093/: 6

Y-Eh /1.35/: -.8

Automatic phase labels? /N/: N

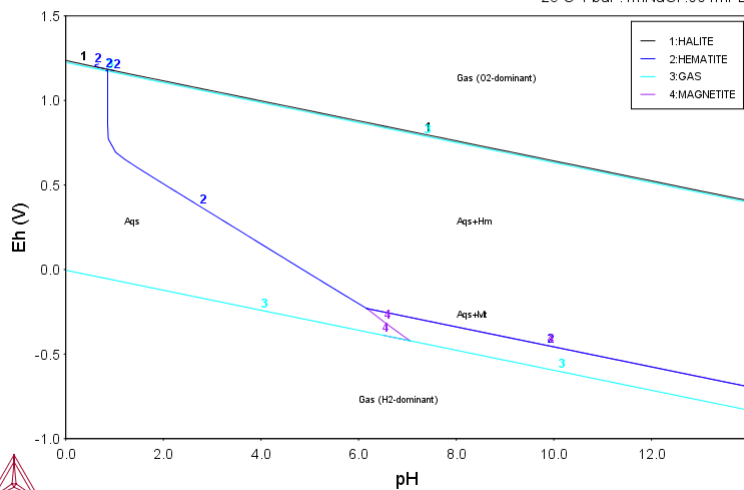
Text? /Aqs/: Gas (H2-dominant)

Text size: /.36/: .26

Another Label Text to be added? /N/: N

2016.05.17.21.33.20  
CL, FE, H+1, NA, H2O, ZE  
T=298.15, P=1E5, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1

25 C 1 bar .1mNaCl .001mFE



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

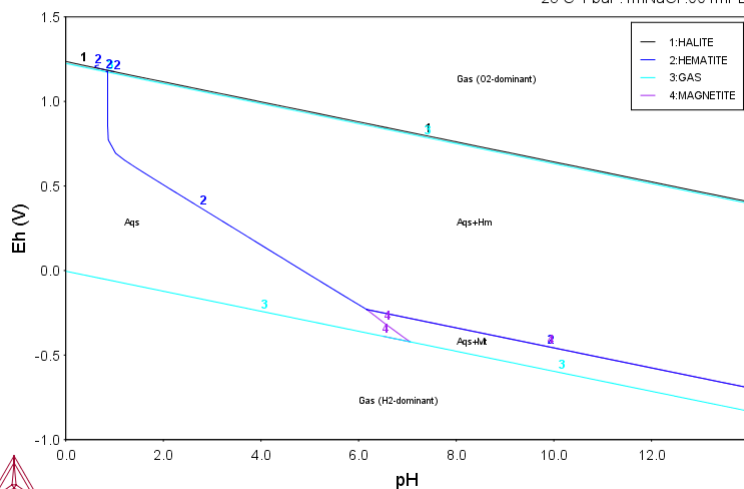
New text /Aqs+Mt/: Aqs+Mt

Another Label Text to be modified? /N/: N

Pourbaix Diagram

2016.05.17.21.33.21  
CL, FE, H+1, NA, H2O, ZE  
T=298.15, P=1E5, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1

25 C 1 bar .1mNaCl .001mFE



Hit RETURN to continue

Modify Label-Curve-Option on the Pourbaix diagram? /N/: y

Curve-Label Option? /E/: ?

THE OPTIONS MEANS:

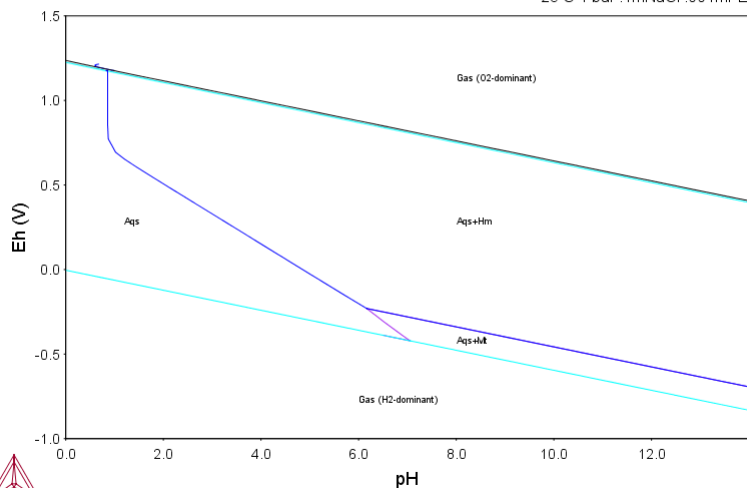
A LIST STABLE PHASES ALONG LINE  
B AS A BUT CURVES WITH SAME FIX PHASE HAVE SAME NUMBER  
C LIST AXIS QUANTITIES  
D AS C BUT CURVES WITH SAME QUANTITIES HAVE SAME NUMBER  
E AS B WITH CHANGING COLORS  
F AS D WITH CHANGING COLORS  
N NO LABELS

CURVE LABEL OPTION (A, B, C, D, E, F OR N) /E/: n

# Pourbaix Diagram

2016.05.17.21.33.21  
CL, FE, H+1, NA, H2O, ZE  
T=298.15, P=1E5, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1

25 C 1 bar .1mNaCl .001mFE



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

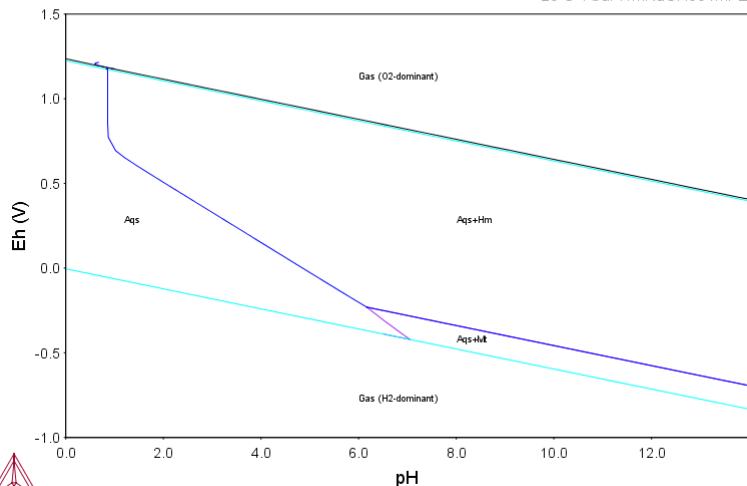
New text /Gas (O2-dominant)/: Gas (O2-dominant)

Another Label Text to be modified? /N/: N

# Pourbaix Diagram

2016.05.17.21.33.22  
CL, FE, H+1, NA, H2O, ZE  
T=298.15, P=1E5, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1

25 C 1 bar .1mNaCl .001mFE



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

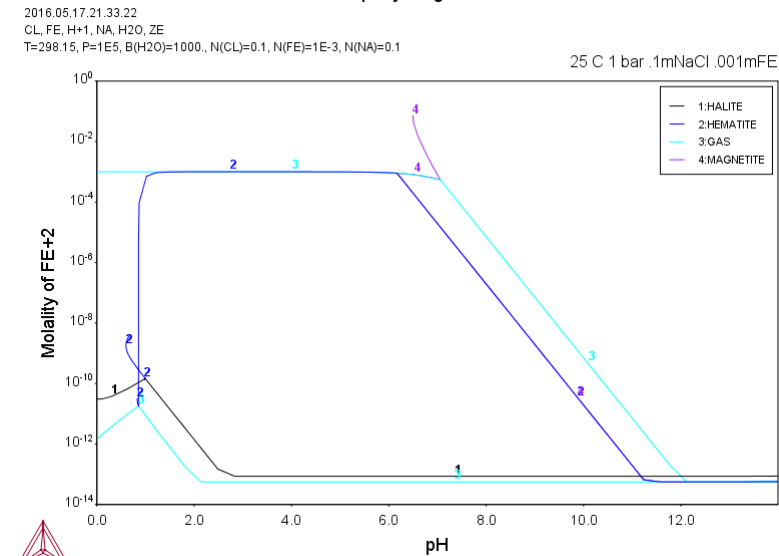
SET PLOTTING PARAMETERS:

-----  
I 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!

Property Diagram



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



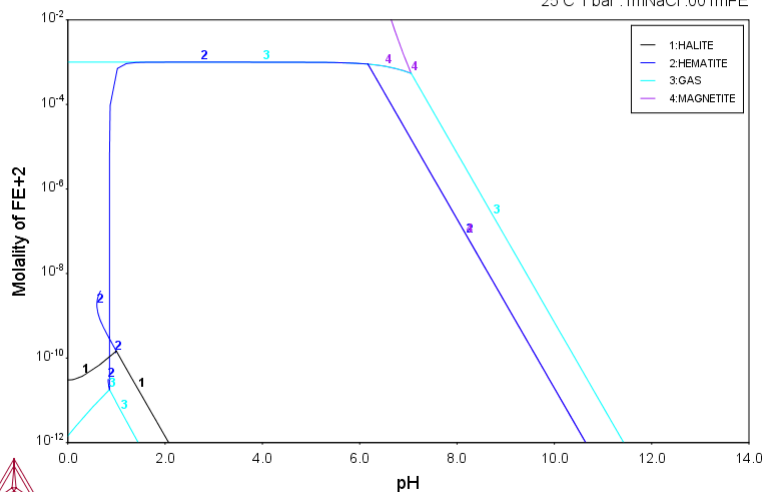
### Property Diagram

2016.05.17.21.33.23

CL, FE, H+1, NA, H2O, ZE

T=298.15, P=1E5, B(H2O)=1000., N(CL)=0.1, N(Fe)=1E-3, N(NA)=0.1

25 C 1 bar .1mNaCl .001mFE



Another zoom? /N/: N

Another zoom? /N/: N

Change Curve-Label Option for the diagram? /N/: N

Add Label-Texts onto the specified diagram? /N/: N

Change the Subtitle of the diagram? /N/: N

Change Axis-Texts? /N/: N

Further Refine the diagram in POST Module? /N/: N

Hard copy of the diagram? /N/: N

Save X-Y coordinates of curve on text file? /N/: N

Modify the diagram? /N/: N

Any more diagram? /N/: y

Loading workspaces from the POLY3 file: POURBAIX

The loaded POLY3 file is of POURBAIX-MAPPING Calculation.

The current system consists of 6 elements:

CL FE H NA O ZE

List of Default and Pre-defined Calculation Conditions:

Units: T in K, P in Pascal, B(H2O) in gram, N(ELEM) in mole

T=298.15, P=1E5, B(H2O)=1000., N(CL)=0.1, N(Fe)=1E-3, N(NA)=0.1,  
LNACR(H+1)=-16.1181, MUR(ZE)=66000.

### FIXED PHASES

FIXED  
CASE-0

DEGREES OF FREEDOM = 1

SET PLOTTING PARAMETERS:

```

I The following properties are available to be selected
I as axis variables for making other diagrams from the
I same calculation:
I
I pH --- Acidity
I Eh --- Electronic Potential (V)
I Ah --- Electronic Affinity (kJ)
I pe --- Electronic Activity (log10ACRe)
I IS --- Ionic Strength
I TM --- Total Concentration
I Aw --- Activity of Water
I Oc --- Osmotic Coefficient
I MF(AQsp) --- Mole Fractions of Aqueous Species
I ML(AQsp) --- Molalities of Aqueous Species
I AI(AQsp) --- Activities of Aqueous Species
I RC(AQsp) --- Activity Coefficients of Aq Species
I
I where "AQsp" is the name of a specific aqueous species,
I and "*" can be used as a wild sign for all "AQsp";
I It is unnecessary to give a complete aqueous species
I names; however, the entered AQsp name must be unique.
I If neither "AQsp" nor "*" is given here, all species
I will be searched.
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

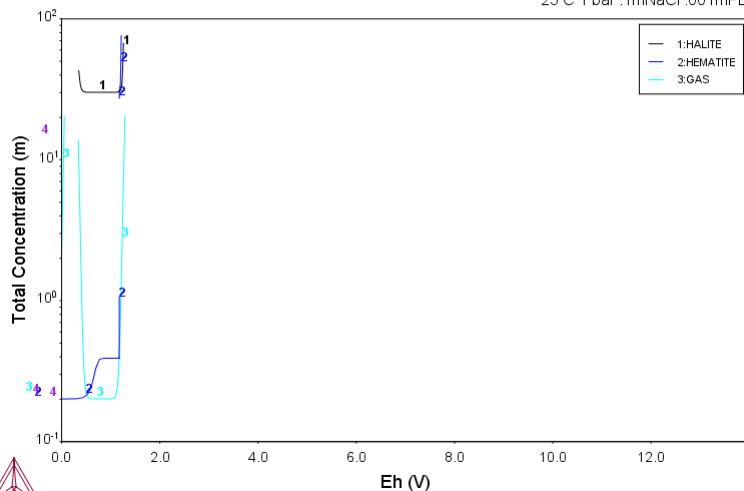
FECL+2	FE03H3-1	FE0H+1	FE0H+2	H+1
H2	H2O	H2O2	HCLO	HCLO2
HO2-1	NA+1	O2	O3	OH-1

X-axis Variable: /PH/: Eh  
Y-axis Variable: /ML/: TM  
CURRENT DEVICE: TC-UNITE Driver  
Plotting the diagram; please be patient!

Property Diagram

2016.05.17.21.33.23  
CL, FE, H+1, NA, H2O, ZE  
T=298.15, P=1E5, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1

25 C 1 bar .1mNaCl .001mFE



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

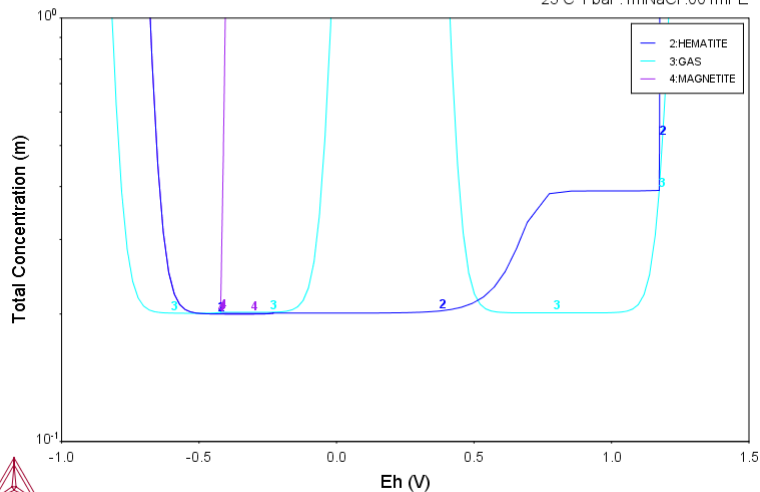
CURRENT DEVICE: TC-UNITE Driver

Plotting the diagram; please be patient!

Property Diagram

2016.05.17.21.33.24  
CL, FE, H+1, NA, H2O, ZE  
T=298.15, P=1E5, B(H2O)=1000., N(CL)=0.1, N(FE)=1E-3, N(NA)=0.1

25 C 1 bar .1mNaCl .001mFE



Hit RETURN to continue

Another zoom? /N/: N

Change Curve-Label Option for the diagram? /N/: N

Add Label-Texts onto the specified diagram? /N/: N

Change the Subtitle of the diagram? /N/: N

Change Axis-Texts? /N/: N

Further Refine the diagram in POST Module? /N/: N

Hard copy of the diagram? /N/: N

Save X-Y coordinates of curve on text file? /N/: N

Modify the diagram? /N/: N

Any more diagram? /N/: N

SYS:

```
SYS: @@... Up to this point, the POURBAIX-module run has accomplished!
SYS:
SYS: @@
SYS: @@ Under MS-Windows, one can optionally use the DOS-command "copy"
SYS: @@ to backup the resulted POURBAIX.POLY3 file as TCEX40.POLY3:
SYS: @@
SYS: @copy POURBAIX.POLY3 TCEX40.POLY3
      1 fil(er) kopierad(e).
SYS:
SYS: SET_INTERACTIVE
... the command in full is SET_INTERACTIVE_MODE
SYS:
```

tcex41

SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software (build 9533) running on WinNT 64-bit wordlength  
Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118  
License library version: 8.5.1.0017  
Linked: Mon May 16 09:31:44 2016

SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex41\tcex41.TCM" set-echo

SYS: @@

SYS: @@

SYS: @@ Calculation of a solubility product

SYS: @@

SYS: set-log ex41,,,

SYS: go p-3

... the command in full is GOTO\_MODULE

POLY version 3.32

POLY\_3: def-mat

... the command in full is DEFINE\_MATERIAL

THERMODYNAMIC DATABASE module

Current database: Steels/Fe-Alloys v8.0

VA DEFINED

L12\_FCC

B2\_BCC

B2\_VACANCY

HIGH\_SIGMA

DICTRA\_FCC\_A1 REJECTED

Database /TCFE8/: tcfe7

Current database: Steels/Fe-Alloys v7.0

VA DEFINED

L12\_FCC

B2\_BCC

B2\_VACANCY

HIGH\_SIGMA

DICTRA\_FCC\_A1 REJECTED

Major element or alloy: fe

Composition input in mass (weight) percent? /Y/:

1st alloying element: c .19

2nd alloying element: mn 1.16

Next alloying element: si .2

Next alloying element: cr .72

Next alloying element: ni .2

Next alloying element: mo .08

Next alloying element: cu .26

Next alloying element: al .027

Next alloying element: n .0089

Next alloying element:

Temperature (C) /1000/: 1056

VA DEFINED

L12\_FCC

B2\_BCC

B2\_VACANCY

HIGH\_SIGMA

DICTRA\_FCC\_A1 REJECTED

REINITIATING GES5 .....

... the command in full is DEFINE\_ELEMENTS

FE DEFINED

... the command in full is DEFINE\_ELEMENTS

C DEFINED

... the command in full is DEFINE\_ELEMENTS

MN DEFINED

... the command in full is DEFINE\_ELEMENTS

SI DEFINED

... the command in full is DEFINE\_ELEMENTS

CR DEFINED

... the command in full is DEFINE\_ELEMENTS

NI DEFINED

... the command in full is DEFINE\_ELEMENTS

MO DEFINED

... the command in full is DEFINE\_ELEMENTS

CU DEFINED

... the command in full is DEFINE\_ELEMENTS

AL DEFINED

... the command in full is DEFINE\_ELEMENTS

N DEFINED

This database has following phases for the defined system

GAS:G	LIQUID:L	BCC_A2
FCC_A1	HCP_A3	DIAMOND_FCC_A4
GRAPHITE	CEMENTITE	M23C6
M7C3	M6C	M5C2
M3C2	MC_ETa	MC_SHP
KSI_CARBIDE	A1_KAPPA	KAPPA
Z_PHASE	FE4N_LP1	FECN_CHI
PI	SIGMA	MU_PHASE
P_PHASE	R_PHASE	CHI_A12
LAVES_PHASE_C14	M3SI	G_PHASE
CR3SI	FE2SI	MSI
M5SI3	NBNI3	NI3TI
AL4C3	FE8SI2C	SIC
ALN	SI3N4	MN6N4
MN6N5		

Reject phase(s) /NONE/: NONE

Restore phase(s): /NONE/: NONE

.....

The following phases are retained in this system:

GAS:G	LIQUID:L	BCC_A2
FCC_A1	HCP_A3	DIAMOND_FCC_A4
GRAPHITE	CEMENTITE	M23C6
M7C3	M6C	M5C2
M3C2	MC_ETa	MC_SHP
KSI_CARBIDE	A1_KAPPA	KAPPA
Z_PHASE	FE4N_LP1	FECN_CHI
PI	SIGMA	MU_PHASE
P_PHASE	R_PHASE	CHI_A12
LAVES_PHASE_C14	M3SI	G_PHASE

CR3SI	FE2SI	MSI
M5SI3	NBNI3	NI3TI
AL4C3	FE8SI2C	SIC
ALN	SI3N4	MN6N4
MN6N5		

.....

OK? /Y/: Y

ELEMENTS .....

SPECIES .....

PHASES .....

... the command in full is AMEND\_PHASE\_DESCRIPTION

... the command in full is AMEND\_PHASE\_DESCRIPTION

... the command in full is AMEND\_PHASE\_DESCRIPTION

... the command in full is AMEND\_PHASE\_DESCRIPTION

... the command in full is AMEND\_PHASE\_DESCRIPTION

PARAMETERS ...

FUNCTIONS ....

List of references for assessed data

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-OK-

**Should any phase have a miscibility gap check? /N/: N**  
 Using global minimization procedure  
 Calculated 29105 grid points in 1 s  
 Found the set of lowest grid points in 0 s  
 Calculated POLY solution 1 s, total time 2 s

**POLY\_3:**  
**POLY\_3:** l-e,,,  
 ... the command in full is LIST\_EQUILIBRIUM  
 Output from POLY-3, equilibrium = 1, label A0 , database: TCFE7

Conditions:  
 T=1329.15, W(C)=1.9E-3, W(MN)=1.16E-2, W(SI)=2E-3, W(CR)=7.2E-3, W(NI)=2E-3,  
 W(MO)=8E-4, W(CU)=2.6E-3, W(AL)=2.7E-4, W(N)=8.9E-5, P=1E5, N=1  
 DEGREES OF FREEDOM 0

Temperature 1329.15 K ( 1056.00 C), Pressure 1.000000E+05  
 Number of moles of components 1.00000E+00, Mass in grams 5.53245E+01  
 Total Gibbs energy -6.89251E+04, Enthalpy 3.91376E+04, Volume 7.33525E-06

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
AL	5.5361E-04	2.7000E-04	1.6468E-09	-2.2351E+05	SER
C	8.7517E-03	1.9000E-03	8.6247E-03	-5.2528E+04	SER
CR	7.6609E-03	7.2000E-03	7.6112E-05	-1.0480E+05	SER
CU	2.2636E-03	2.6000E-03	1.0015E-04	-1.0177E+05	SER
FE	9.6245E-01	9.7154E-01	2.2979E-03	-6.7145E+04	SER
MN	1.1682E-02	1.1600E-02	1.1078E-05	-1.2610E+05	SER
MO	4.6133E-04	8.0000E-04	9.9033E-06	-1.2734E+05	SER
N	3.5153E-04	8.9000E-05	5.1545E-07	-1.6000E+05	SER
NI	1.8853E-03	2.0000E-03	2.7230E-06	-1.4161E+05	SER
SI	3.9396E-03	2.0000E-03	5.2580E-09	-2.1068E+05	SER

FCC\_A1 Status ENTERED Driving force 0.0000E+00  
 Moles 9.9974E-01, Mass 5.5319E+01, Volume fraction 9.9977E-01 Mass fractions:  
 FE 9.71636E-01 CU 2.60025E-03 C 1.90019E-03 N 5.57073E-05  
 MN 1.16011E-02 SI 2.00019E-03 MO 8.00078E-04

```

CR 7.20070E-03 NI 2.00019E-03 AL 2.05877E-04

ALN Status ENTERED Driving force 0.0000E+00
Moles 2.6304E-04, Mass 5.3909E-03, Volume fraction 2.2895E-04 Mass fractions:
AL 6.58274E-01 NI 0.00000E+00 FE 0.00000E+00 C 0.00000E+00
N 3.41726E-01 MO 0.00000E+00 CU 0.00000E+00
SI 0.00000E+00 MN 0.00000E+00 CR 0.00000E+00
POLY_3:Hit RETURN to continue
POLY_3:
POLY_3: def-dia
... the command in full is DEFINE_DIAGRAM
Same elements as before? /Y/: Y
For binary or ternary diagrams you may prefer the special modules

You must specify a value for all compositions and the temperature even
if you want to use it as axis.
Mass (weight) percent of AL /.027/: .027
Mass (weight) percent of C /.19/: .19
Mass (weight) percent of CR /.72/: .72
Mass (weight) percent of CU /.26/: .26
Mass (weight) percent of MN /1.16/: 1.16
Mass (weight) percent of MO /.08/: .08
Mass (weight) percent of N /.0089/: .0089
Mass (weight) percent of NI /.2/: .2
Mass (weight) percent of SI /.2/: .2
Temperature (C) /1056/: 1056
Using global minimization procedure
Using already calculated grid
Found the set of lowest grid points in 0 s
Calculated POLY solution 1 s, total time 1 s
You must now set an independent axis for your diagram
as one of the following conditions:
Condition 1 is temperature (Celsius)
Condition 2 is mass percent of C
Condition 3 is mass percent of MN
Condition 4 is mass percent of SI
Condition 5 is mass percent of CR
Condition 6 is mass percent of NI
Condition 7 is mass percent of MO
Condition 8 is mass percent of CU
Condition 9 is mass percent of AL
Condition 10 is mass percent of N
Give the number of the condition to vary /1/: 1
Minimum value (C) /800/: 650
Maximum value (C) /1800/: 1200

The second axis can be another of the conditions above and you will then
calculate a phase diagram.
Or you may want to plot how some other quantities depend on the selected
condition and you will then calculate a "property" diagram.

In addition to the conditions above you may use these selected
dependent quantities on the vertical axis:
Dependent 11 is mass fraction of all phases
Dependent 12 is composition of a phase
Dependent 13 is the fraction of a component in all phases
(In the post processor you may select many other quantities)
Give the number of the quantity on second axis /11/: 11 tcex41
No initial equilibrium, using default
Step will start from axis value 1329.15
...OK

Phase Region from 1329.15 for:
ALN
FCC_A1
Global Check of removing phase at 1.38422E+03
Calculated 8 equilibria

Phase Region from 1384.22 for:
FCC_A1
Global Test at 1.45915E+03 .... OK
Terminating at 1473.15
Calculated 13 equilibria

Phase Region from 1329.15 for:
ALN
FCC_A1
Global Test at 1.24915E+03 .... OK
Global test at 1.14915E+03 .... OK
Global check of adding phase at 1.07227E+03
Calculated 28 equilibria

Phase Region from 1072.27 for:
ALN
BCC_A2
FCC_A1
Global Test at 9.99150E+02 .... OK
Global check of adding phase at 9.98511E+02
Calculated 11 equilibria

Phase Region from 998.511 for:
ALN
BCC_A2
FCC_A1
M7C3
Global check of adding phase at 9.96944E+02
Calculated 3 equilibria

Phase Region from 996.944 for:
ALN
BCC_A2
CEMENTITE
FCC_A1
M7C3
Global check of removing phase at 9.95944E+02
Calculated 3 equilibria

Phase Region from 995.944 for:
ALN
BCC_A2
CEMENTITE
FCC_A1
Global check of removing phase at 9.68325E+02
Calculated 6 equilibria

```

```

Phase Region from 968.325 for:
  ALN
  BCC_A2
  CEMENTITE
Global check of adding phase at 9.45779E+02
Calculated 5 equilibria

Phase Region from 945.779 for:
  ALN
  BCC_A2
  CEMENTITE
  M7C3
Terminating at 923.150
Calculated 6 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex41\tcex
41.POLY3

```

POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

... the command in full is REINITIATE\_PLOT\_SETTINGS

POSTPROCESSOR VERSION 3.2

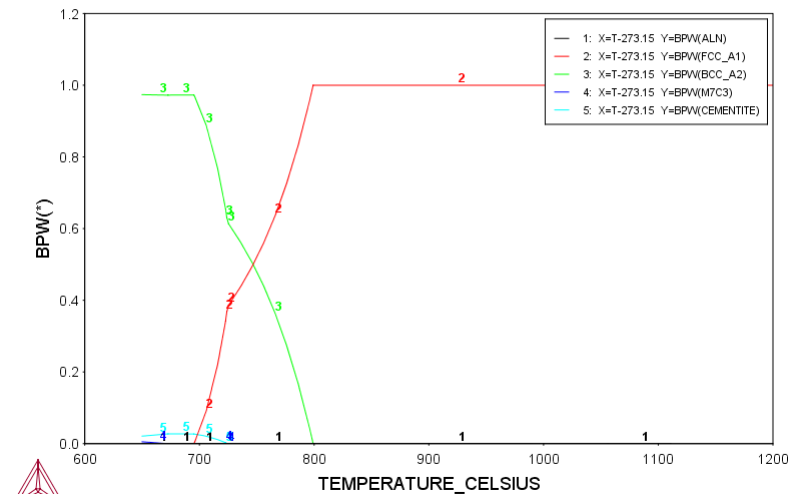
Setting automatic diagram axes

... the command in full is SET\_AUTOMATIC\_DIAGRAM\_A

Setting automatic diagram axes

... the command in full is PLOT DIAGRAM

2016.05.16.14.31.12  
TCFE7: AL, C, CR, CU, FE, MN, MO, N, NI, SI  
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.



```

POST:
POST:Hit RETURN to continue
POST:
POST: s-d-a x w(fcc,al)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y w(fcc,n)
... the command in full is SET_DIAGRAM_AXIS
POST:
POST: s-d-a z t
... the command in full is SET_DIAGRAM_AXIS
POST: s-s z n 1250 1350
... the command in full is SET_SCALING_STATUS
POST:
POST: set-title example 41a
POST: plot
... the command in full is PLOT_DIAGRAM

```

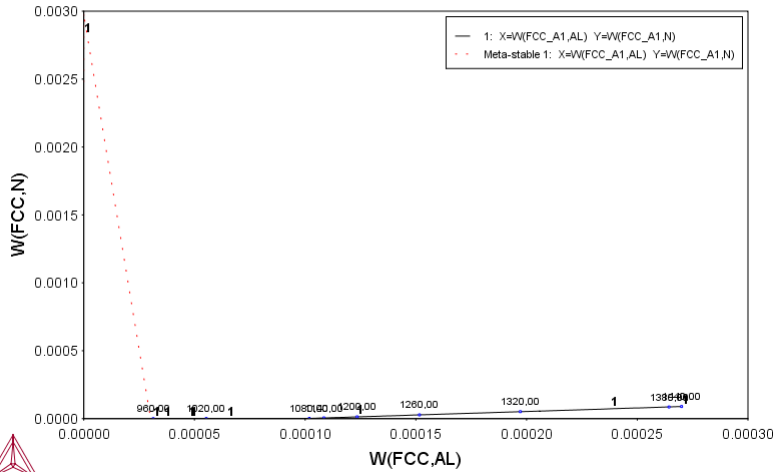


### example 41a

2016.05.16.14.31.13

TCFE7: AL, C, CR, CU, FE, MN, MO, N, NI, SI

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.



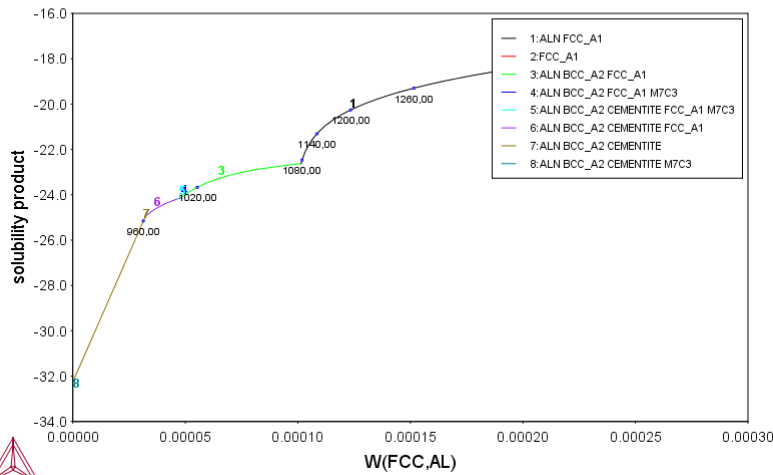
```
POST:
POST:
POST:Hit RETURN to continue
POST: @@ Now let's go back to POLY3 and enter a function
POST: @@ corresponding to the solubility product
POST: back
POLY_3: enter fun
... the command in full is ENTER_SYMBOL
Name: sp
Function: log(w(fcc,al)*w(fcc,n));
POLY_3:
POLY_3: @@ Finally, let's go back to POST and plot the entered function
POLY_3: post
POST:
POST: s-d-a y sp
... the command in full is SET_DIAGRAM_AXIS
POST: s-lab b
... the command in full is SET_LABEL_CURVE_OPTION
POST: s-a-t-s y n solubility product
... the command in full is SET_AXIS_TEXT_STATUS
POST:
POST: set-title example 41b
POST:
POST: plot
... the command in full is PLOT DIAGRAM
```

### example 41b

2016.05.16.14.31.14

TCFE7: AL, C, CR, CU, FE, MN, MO, N, NI, SI

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.



```
POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:
```

About Stockholm, Sweden

Software (build 9533) running on WinNT 64-bit wordlength  
Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118  
License library version: 8.5.1.0017  
Linked: Mon May 16 09:31:44 2016

SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex42\tcex42.TCM"SYS: set-echo

SYS: @@  
SYS: @@  
SYS: @@ Paraequilibrium calculation - Formation of Para-pearlite - Isopleth  
SYS: @@  
SYS: @@ Fe-Mn-C system at 2.5%Mn Mass u-fraction  
SYS: @@  
SYS: set-log ex42,,,  
SYS: go da  
... the command in full is GOTO\_MODULE  
THERMODYNAMIC DATABASE module  
Current database: Steels/Fe-Alloys v8.0

VA DEFINED  
L12\_FCC B2\_BCC B2\_VACANCY  
HIGH\_SIGMA DICTRA\_FCC\_A1 REJECTED  
TDB\_TCFE8: sw tcfe7  
... the command in full is SWITCH\_DATABASE  
Current database: Steels/Fe-Alloys v7.0

VA DEFINED  
L12\_FCC B2\_BCC B2\_VACANCY  
HIGH\_SIGMA DICTRA\_FCC\_A1 REJECTED  
TDB\_TCFE7: d-sys fe c mn  
... the command in full is DEFINE\_SYSTEM  
FE C MN

DEFINED  
TDB\_TCFE7: rej ph gra m5c2  
... the command in full is REJECT  
GRAPHITE M5C2 REJECTED  
TDB\_TCFE7: get  
... the command in full is GET\_DATA  
REINITIATING GES5 .....  
ELEMENTS .....  
SPECIES .....  
PHASES .....  
... the command in full is AMEND\_PHASE\_DESCRIPTION  
... the command in full is AMEND\_PHASE\_DESCRIPTION  
... the command in full is AMEND\_PHASE\_DESCRIPTION  
... the command in full is AMEND\_PHASE\_DESCRIPTION  
... the command in full is AMEND\_PHASE\_DESCRIPTION  
PARAMETERS ...  
FUNCTIONS ....

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'B. Uhrenius (1993-1994), International journal of refractory metals and hard mater, Vol. 12, pp. 121-127; Molar volumes'  
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'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'  
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'N. Saunders, COST 507 Report (1998); Mn-Ti'  
'A. Markstrom, Thermo-Calc software AB, 2011'  
-OK-

TDB\_TCFE7: go p-3  
... the command in full is GOTO\_MODULE

POLY version 3.32  
POLY\_3: @@  
POLY\_3: @@ To work with u-fractions, simply set the status of component C to SPECIAL  
POLY\_3: @@  
POLY\_3: c-s com c  
... the command in full is CHANGE\_STATUS  
Status: /ENTERED/: special  
POLY\_3: l-st  
... the command in full is LIST\_STATUS  
Option /CPS/:

*** STATUS FOR ALL COMPONENTS				
COMPONENT	STATUS	REF. STATE	T(K)	P(Pa)
VA	ENTERED	SER		
C	SPECIAL	SER		
FE	ENTERED	SER		
MN	ENTERED	SER		
*** STATUS FOR ALL PHASES				
PHASE	STATUS	DRIVING FORCE	MOLES	
M7C3	ENTERED	0.000000E+00	0.000000E+00	
M23C6	ENTERED	0.000000E+00	0.000000E+00	
LAVES_PHASE_C14	ENTERED	0.000000E+00	0.000000E+00	
KSI_CARBIDE	ENTERED	0.000000E+00	0.000000E+00	

```

KAPPA          ENTERED      0.000000E+00    0.000000E+00
HCP_A3         ENTERED      0.000000E+00    0.000000E+00
G_PHASE        ENTERED      0.000000E+00    0.000000E+00
FECN_CHI       ENTERED      0.000000E+00    0.000000E+00
FE4N_LP1       ENTERED      0.000000E+00    0.000000E+00
FCC_A1         ENTERED      0.000000E+00    0.000000E+00
DIAMOND_FCC_A4 ENTERED      0.000000E+00    0.000000E+00
CEMENTITE      ENTERED      0.000000E+00    0.000000E+00
BCC_A2         ENTERED      0.000000E+00    0.000000E+00
LIQUID         ENTERED      0.000000E+00    0.000000E+00
GAS            ENTERED      0.000000E+00    0.000000E+00
*** STATUS FOR ALL SPECIES
C   ENTERED   C3  ENTERED   C5  ENTERED   FE  ENTERED   VA  ENTERED
C2  ENTERED   C4  ENTERED   C60 ENTERED   MN  ENTERED

POLY_3:
POLY_3:Hit RETURN to continue
POLY_3: s-c t=900 p=1e5 n=1 w(c)=0.002 w(mn)=0.025
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      13031 grid points in      0 s
Found the set of lowest grid points in      0 s
Calculated POLY solution      0 s, total time      0 s
POLY_3: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
Output from POLY-3, equilibrium =      1, label A0 , database: TCFE7

Conditions:
T=900, P=1E5, N=1, W(C)=2E-3, W(MN)=2.5E-2
DEGREES OF FREEDOM 0

Temperature      900.00 K (      626.85 C), Pressure      1.000000E+05
Number of moles of components      1.000000E+00, Mass in grams      5.54204E+01
Total Gibbs energy -3.64282E+04, Enthalpy      2.02873E+04, Volume      7.24808E-06

Component      Moles      W-Fraction Activity Potential Ref.stat
C      9.2099E-03      2.0000E-03      1.8066E-01      -1.2805E+04 SER
FE      9.6562E-01      9.7500E-01      8.1690E-03      -3.5974E+04 SER
MN      2.5169E-02      2.5000E-02      2.3600E-04      -6.2496E+04 SER

BCC_A2          Status ENTERED      Driving force      0.0000E+00
Moles 9.6371E-01, Mass 5.3798E+01, Volume fraction 9.6995E-01 Mass fractions:
FE 9.81636E-01 MN 1.83337E-02 C 3.07634E-05

CEMENTITE          Status ENTERED      Driving force      0.0000E+00
Moles 3.6288E-02, Mass 1.6223E+00, Volume fraction 3.0048E-02 Mass fractions:
FE 6.88481E-01 MN 2.4435E-01 C 6.71647E-02
POLY_3: s-a-v 1 w(c) 0 0.02
... the command in full is SET_AXIS_VARIABLE
Increment /5E-04/: 2.5E-04
POLY_3: s-a-v 2 t 800 1200 10
... the command in full is SET_AXIS_VARIABLE
POLY_3: sa tcex42a y
... the command in full is SAVE_WORKSPACES
POLY_3: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Tie-lines not in the plane of calculation
Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28
Generating start point 29
Generating start point 30
Working hard
Working hard

Phase region boundary 1 at:      2.500E-04      8.868E+02
      BCC_A2
      CEMENTITE

```

```

** FCC_A1
Calculated.                3  equilibria

Phase region boundary  2 at:  1.756E-05  8.799E+02
  BCC_A2
** CEMENTITE
** FCC_A1

Phase region boundary  3 at:  1.756E-05  8.799E+02
  BCC_A2
** FCC_A1
Calculated.                18  equilibria

Phase region boundary  4 at:  1.756E-05  8.799E+02
  BCC_A2
** CEMENTITE
Calculated..              10  equilibria
Terminating at axis limit.

Phase region boundary  5 at:  1.756E-05  8.799E+02
  BCC_A2
** CEMENTITE
  FCC_A1
Calculated.                34  equilibria

Phase region boundary  6 at:  6.887E-03  9.767E+02
** BCC_A2
** CEMENTITE
  FCC_A1

Phase region boundary  7 at:  6.887E-03  9.767E+02
** CEMENTITE
  FCC_A1
Calculated..              37  equilibria
Terminating at axis limit.

Phase region boundary  8 at:  6.887E-03  9.767E+02
** BCC_A2
  FCC_A1
Calculated.                47  equilibria

Phase region boundary  9 at:  6.887E-03  9.767E+02
** BCC_A2
  CEMENTITE
  FCC_A1
Calculated..              54  equilibria
Terminating at axis limit.

Phase region boundary 10 at:  1.756E-05  8.799E+02
  BCC_A2
  CEMENTITE
** FCC_A1
Calculated..              85  equilibria
Terminating at axis limit.

Phase region boundary 11 at:  2.500E-04  8.868E+02
  BCC_A2
  CEMENTITE
** FCC_A1
Calculated..              81  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 12 at:  6.750E-03  9.510E+02
  BCC_A2
  CEMENTITE
** FCC_A1
Calculated.                29  equilibria
Terminating at known equilibrium

Phase region boundary 13 at:  6.750E-03  9.510E+02
  BCC_A2
  CEMENTITE
** FCC_A1
Calculated..              55  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 14 at:  1.325E-02  9.678E+02
  BCC_A2
  CEMENTITE
** FCC_A1
Calculated.                57  equilibria
Terminating at known equilibrium

Phase region boundary 15 at:  1.325E-02  9.678E+02
  BCC_A2
  CEMENTITE
** FCC_A1
Calculated..              29  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 16 at:  3.686E-06  8.100E+02
  BCC_A2
** CEMENTITE
Calculated..              3  equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 17 at:  3.686E-06  8.100E+02
  BCC_A2
** CEMENTITE
Calculated.                8  equilibria
Terminating at known equilibrium

Phase region boundary 18 at:  1.975E-02  9.759E+02
  BCC_A2
  CEMENTITE
** FCC_A1
Calculated.               80  equilibria
Terminating at known equilibrium

Phase region boundary 19 at:  1.975E-02  9.759E+02
  BCC_A2
  CEMENTITE

```

```

** FCC_A1
Calculated.. 3 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 20 at: 1.114E-03 9.367E+02
BCC_A2
** CEMENTITE
FCC_A1
Calculated. 8 equilibria
Terminating at known equilibrium

Phase region boundary 21 at: 1.114E-03 9.367E+02
BCC_A2
** CEMENTITE
FCC_A1
Calculated. 26 equilibria
Terminating at known equilibrium

Phase region boundary 22 at: 4.017E-03 9.367E+02
BCC_A2
CEMENTITE
** FCC_A1
Calculated. 17 equilibria
Terminating at known equilibrium

Phase region boundary 23 at: 4.017E-03 9.367E+02
BCC_A2
CEMENTITE
** FCC_A1
Calculated.. 66 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 24 at: 1.018E-03 1.063E+03
** BCC_A2
FCC_A1
Calculated. 32 equilibria
Terminating at known equilibrium

Phase region boundary 25 at: 1.018E-03 1.063E+03
** BCC_A2
FCC_A1
Calculated 17 equilibria

Phase region boundary 26 at: 9.139E-03 1.063E+03
** CEMENTITE
FCC_A1
Calculated. 10 equilibria
Terminating at known equilibrium

Phase region boundary 27 at: 9.139E-03 1.063E+03
** CEMENTITE
FCC_A1
Calculated.. 28 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 28 at: 1.283E-02 1.190E+03
** CEMENTITE
FCC_A1
Calculated. 34 equilibria
Terminating at known equilibrium

Phase region boundary 29 at: 1.283E-02 1.190E+03
** CEMENTITE
FCC_A1
Calculated.. 4 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 30 at: 2.500E-04 1.081E+03
** BCC_A2
FCC_A1
Calculated 4 equilibria

Phase region boundary 31 at: 2.500E-04 1.081E+03
** BCC_A2
FCC_A1
Calculated. 28 equilibria
Terminating at known equilibrium

Phase region boundary 32 at: 6.750E-03 9.783E+02
** BCC_A2
FCC_A1
Calculated 30 equilibria

Phase region boundary 33 at: 6.750E-03 9.783E+02
** BCC_A2
FCC_A1
Calculated. 2 equilibria
Terminating at known equilibrium

Phase region boundary 34 at: 1.325E-02 9.803E+02
** BCC_A2
CEMENTITE
FCC_A1
Calculated. 27 equilibria
Terminating at known equilibrium

Phase region boundary 35 at: 1.325E-02 9.803E+02
** BCC_A2
CEMENTITE
FCC_A1
Calculated.. 29 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 36 at: 1.283E-02 1.190E+03
** CEMENTITE
FCC_A1
Calculated. 34 equilibria
Terminating at known equilibrium

Phase region boundary 37 at: 1.283E-02 1.190E+03
** CEMENTITE

```

```

FCC_A1
Calculated.. 4 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 38 at: 1.975E-02 9.830E+02
** BCC_A2
CEMENTITE
FCC_A1
Calculated. 53 equilibria
Terminating at known equilibrium

Phase region boundary 39 at: 1.975E-02 9.830E+02
** BCC_A2
CEMENTITE
FCC_A1
Calculated.. 3 equilibria
Terminating at known equilibrium
Terminating at axis limit.
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex42\tcex
42a.POLY3
CPU time for mapping 7 seconds
POLY_3: po
... the command in full is POST

POLY-3 POSTPROCESSOR VERSION 3.2

```

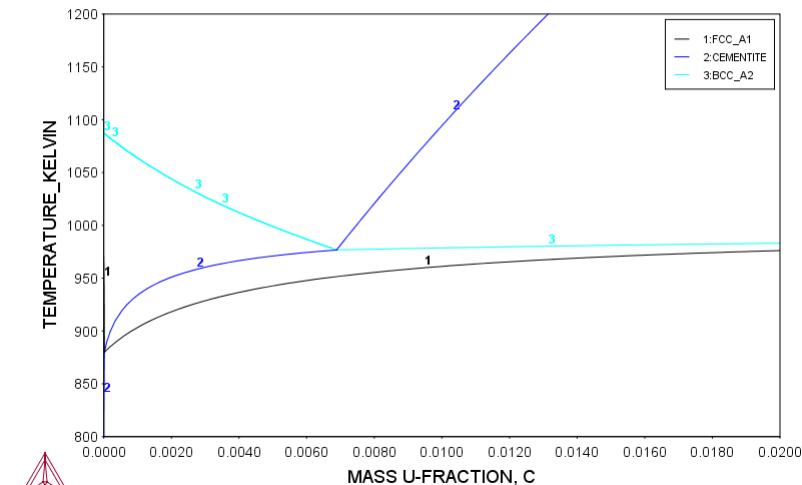
```

Setting automatic diagram axes

POST: s-lab e
... the command in full is SET_LABEL_CURVE_OPTION
POST: s-a-text x n MASS U-FRACTION, C
... the command in full is SET_AXIS_TEXT_STATUS
POST: set-title example 42a
POST:
POST: plot
... the command in full is PLOT DIAGRAM

```

2016.05.16.14.33.09  
TCFE7: C, FE, MN  
P=1E5, N=1, W(MN)=2.5E-2



```

POST:
POST:Hit RETURN to continue
POST:
POST: make tcex42 y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST:
POST: back
POLY_3: read tcex42a
... the command in full is READ_WORKSPACES
POLY_3: s-a-v 1 t 800 1200 10
... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 none
... the command in full is SET_AXIS_VARIABLE
POLY_3: sa tcex42b y
... the command in full is SAVE_WORKSPACES
POLY_3: step
... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: para

```

This command calculates a paraequilibrium between two phases.  
You must calculate an equilibrium with the overall composition first.

```

Name of first phase: fcc_a1
Name of second phase: bcc_a2
Fast diffusing component: /C/: C
Fast diffusing component: /NONE/:

```

Output during stepping is:  
axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,  
and LNACR value(s) of interstitial(s)

Phase Region from	900.000	for:				
BCC_A2						
FCC_A1						
9.000000E+02	0.176	0.824	4.977501E-02	6.609390E-04	-2.303643E-01	
8.900000E+02	0.161	0.839	5.421135E-02	6.889794E-04	-1.689777E-02	
8.800000E+02	0.148	0.852	5.872152E-02	7.140931E-04	1.943989E-01	
8.700000E+02	0.137	0.863	6.329608E-02	7.362105E-04	4.040959E-01	
8.600000E+02	0.127	0.873	6.792661E-02	7.552871E-04	6.126989E-01	
8.500000E+02	0.119	0.881	7.260558E-02	7.713010E-04	8.206607E-01	
8.400000E+02	0.111	0.889	7.732629E-02	7.842505E-04	1.028392E+00	
8.300000E+02	0.105	0.895	8.208278E-02	7.941530E-04	1.236267E+00	
8.200000E+02	0.099	0.901	8.686971E-02	8.010431E-04	1.444633E+00	
8.100000E+02	0.093	0.907	9.168236E-02	8.049714E-04	1.653814E+00	

```

8.000000E+02    0.089    0.911    9.651648E-02    8.060032E-04    1.864114E+00
Phase Region from    900.000    for:
  BCC_A2
  FCC_A1
9.000000E+02    0.176    0.824    4.977501E-02    6.609390E-04    -2.303643E-01
9.100000E+02    0.193    0.807    4.542308E-02    6.300692E-04    -4.466511E-01
9.200000E+02    0.214    0.786    4.116735E-02    5.964982E-04    -6.665081E-01
9.300000E+02    0.240    0.760    3.702095E-02    5.603899E-04    -8.908100E-01
9.400000E+02    0.270    0.730    3.299845E-02    5.219482E-04    -1.120589E+00
9.500000E+02    0.308    0.692    2.911596E-02    4.814238E-04    -1.357076E+00
9.600000E+02    0.355    0.645    2.539121E-02    4.391211E-04    -1.601760E+00
9.700000E+02    0.415    0.585    2.184354E-02    3.954079E-04    -1.856463E+00
9.800000E+02    0.493    0.507    1.849394E-02    3.507265E-04    -2.123436E+00
9.900000E+02    0.597    0.403    1.536496E-02    3.056079E-04    -2.405499E+00
1.000000E+03    0.739    0.261    1.248054E-02    2.606888E-04    -2.706208E+00
1.010000E+03    0.942    0.058    9.852896E-03    2.164281E-04    -3.031479E+00
1.020000E+03    1.259    -0.259    7.420594E-03    1.715531E-04    -3.400603E+00
1.030000E+03    1.821    -0.821    5.161354E-03    1.256551E-04    -3.846325E+00
1.040000E+03    3.087    -2.087    3.063915E-03    7.858616E-05    -4.447717E+00
1.050000E+03    8.516    -7.516    1.118169E-03    3.022614E-05    -5.532996E+00
*** Buffer savend on file
c:\jenkins\WORKSP~1\THERMO~1\examples\tcex42\TCEX42~2.POL

```

```

*** ERROR      8 IN NS01AD
*** Numerical error

```

```

POLY_3:
POLY_3: post

```

```

POLY-3 POSTPROCESSOR VERSION 3.2

```

```

Setting automatic diagram axes

```

```

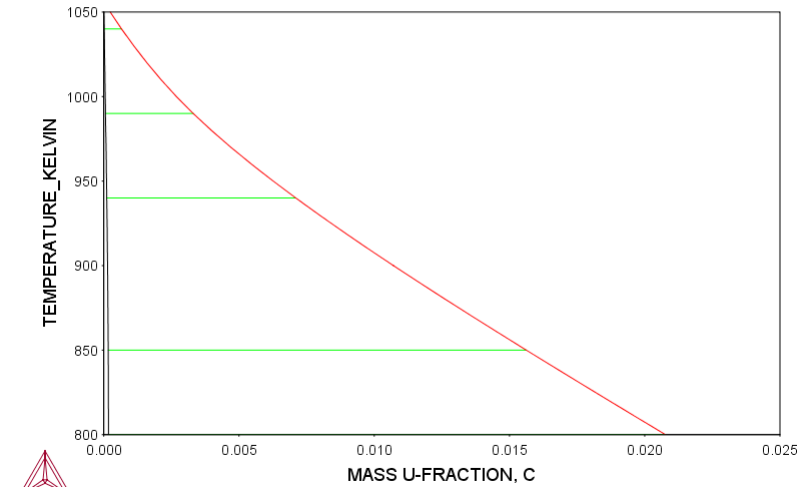
POST: s-d-a x w(*,c)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: s-d-a y t-k
... the command in full is SET_DIAGRAM_AXIS
POST: s-a-text x n MASS U-FRACTION, C
... the command in full is SET_AXIS_TEXT_STATUS
POST: set-tie 5
... the command in full is SET_TIELINE_STATUS
POST: set-title example 42b
POST:
POST: plot
... the command in full is PLOT_DIAGRAM
                                example 42b

```

```

2016.05.16.14.33.11
TCFE7: C, FE, MN
P=1E5, N=1, W(C)=2E-3, W(MN)=2.5E-2

```



```

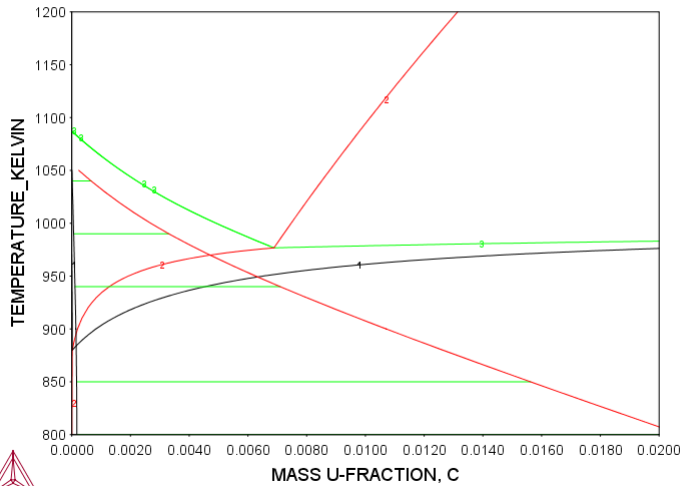
POST:
POST:Hit RETURN to continue
POST:
POST: ap-e y tcex42
... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: s-s x n 0 0.02
... the command in full is SET_SCALING_STATUS
POST: s-s y n 800 1200
... the command in full is SET_SCALING_STATUS
POST: set-title example 42c
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

# example 42c

2016.05.16.14.33.11  
TCFE7: C, FE, MN  
P=1E5, N=1, W(C)=2E-3, W(MN)=2.5E-2

1\*FCC\_A1  
2\*CEMENTITE  
3\*BCC\_A2



POST:Hit RETURN to continue

POST:

POST: back

POLY\_3: read tcex42b

... the command in full is READ\_WORKSPACES

POLY\_3: s-c w(c)=0.01

... the command in full is SET\_CONDITION

POLY\_3: c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Using global minimization procedure

Calculated 13031 grid points in 0 s

Found the set of lowest grid points in 0 s

Calculated POLY solution 0 s, total time 0 s

POLY\_3: l-e

... the command in full is LIST\_EQUILIBRIUM

OUTPUT TO SCREEN OR FILE /SCREEN/:

Options /VWCS/:

Output from POLY-3, equilibrium = 1, label A0 , database: TCFE7

Conditions:

T=900, P=1E5, N=1, W(C)=1E-2, W(MN)=2.5E-2

DEGREES OF FREEDOM 0

Temperature 900.00 K ( 626.85 C), Pressure 1.000000E+05

Number of moles of components 1.00000E+00, Mass in grams 5.38780E+01

Total Gibbs energy -3.55135E+04, Enthalpy 2.04087E+04, Volume 7.05542E-06

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
C	4.4413E-02	1.0000E-02	2.8953E-01	-9.2753E+03	SER
FE	9.3131E-01	9.7500E-01	8.2548E-03	-3.5896E+04	SER
MN	2.4275E-02	2.5000E-02	1.0105E-04	-6.8844E+04	SER

BCC\_A2 Status ENTERED Driving force 0.0000E+00

Moles 8.2304E-01, Mass 4.5951E+01, Volume fraction 8.4974E-01 Mass fractions:

FE 9.92487E-01 MN 7.46758E-03 C 4.52842E-05

CEMENTITE Status ENTERED Driving force 0.0000E+00

Moles 1.7696E-01, Mass 7.9270E+00, Volume fraction 1.5026E-01 Mass fractions:

FE 8.08018E-01 MN 1.24950E-01 C 6.70326E-02

POLY\_3:

POLY\_3: step

... the command in full is STEP\_WITH\_OPTIONS

Option? /NORMAL/: para

This command calculates a paraequilibrium between two phases.

You must calculate an equilibrium with the overall composition first.

Name of first phase: fcc\_a1

Name of second phase: cementite

Fast diffusing component: /C/: C

Fast diffusing component: /NONE/:

Output during stepping is:

axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,  
and LNACR value(s) of interstitial(s)

Phase	Region	from	900.000	for:					
CEMENTITE	FCC_A1								
		9.000000E+02	0.932	0.068	2.554923E-02	3.333333E-01	-1.148376E+00		
		8.900000E+02	0.929	0.071	2.453374E-02	3.333333E-01	-1.120519E+00		
		8.800000E+02	0.926	0.074	2.353422E-02	3.333333E-01	-1.092268E+00		
		8.700000E+02	0.923	0.077	2.255097E-02	3.333333E-01	-1.063621E+00		
		8.600000E+02	0.920	0.080	2.158434E-02	3.333333E-01	-1.034574E+00		
		8.500000E+02	0.917	0.083	2.063468E-02	3.333333E-01	-1.005126E+00		
		8.400000E+02	0.915	0.085	1.970236E-02	3.333333E-01	-9.752721E-01		
		8.300000E+02	0.912	0.088	1.878777E-02	3.333333E-01	-9.450113E-01		
		8.200000E+02	0.909	0.091	1.789129E-02	3.333333E-01	-9.143405E-01		
		8.100000E+02	0.907	0.093	1.701335E-02	3.333333E-01	-8.832577E-01		
		8.000000E+02	0.904	0.096	1.615437E-02	3.333333E-01	-8.517606E-01		

Phase	Region	from	900.000	for:					
CEMENTITE	FCC_A1								
		9.000000E+02	0.932	0.068	2.554923E-02	3.333333E-01	-1.148376E+00		
		9.100000E+02	0.935	0.065	2.658037E-02	3.333333E-01	-1.175842E+00		
		9.200000E+02	0.938	0.062	2.762688E-02	3.333333E-01	-1.202921E+00		
		9.300000E+02	0.942	0.058	2.868849E-02	3.333333E-01	-1.229615E+00		
		9.400000E+02	0.945	0.055	2.976496E-02	3.333333E-01	-1.255928E+00		
		9.500000E+02	0.948	0.052	3.085606E-02	3.333333E-01	-1.281861E+00		
		9.600000E+02	0.952	0.048	3.196156E-02	3.333333E-01	-1.307420E+00		
		9.700000E+02	0.955	0.045	3.308128E-02	3.333333E-01	-1.332605E+00		
		9.800000E+02	0.959	0.041	3.421503E-02	3.333333E-01	-1.357420E+00		
		9.900000E+02	0.963	0.037	3.536265E-02	3.333333E-01	-1.381869E+00		



1.000000E+03	0.966	0.034	3.652401E-02	3.333333E-01	-1.405953E+00
1.010000E+03	0.970	0.030	3.769896E-02	3.333333E-01	-1.429677E+00
1.020000E+03	0.974	0.026	3.888741E-02	3.333333E-01	-1.453041E+00
1.030000E+03	0.978	0.022	4.008925E-02	3.333333E-01	-1.476050E+00
1.040000E+03	0.982	0.018	4.130440E-02	3.333333E-01	-1.498705E+00
1.050000E+03	0.986	0.014	4.253282E-02	3.333333E-01	-1.521010E+00
1.060000E+03	0.991	0.009	4.377444E-02	3.333333E-01	-1.542967E+00
1.070000E+03	0.995	0.005	4.502924E-02	3.333333E-01	-1.564577E+00
1.080000E+03	0.999	0.001	4.629720E-02	3.333333E-01	-1.585844E+00
1.090000E+03	1.004	-0.004	4.757831E-02	3.333333E-01	-1.606770E+00
1.100000E+03	1.008	-0.008	4.887260E-02	3.333333E-01	-1.627357E+00
1.110000E+03	1.013	-0.013	5.018009E-02	3.333333E-01	-1.647607E+00
1.120000E+03	1.018	-0.018	5.150082E-02	3.333333E-01	-1.667522E+00
1.130000E+03	1.023	-0.023	5.283486E-02	3.333333E-01	-1.687104E+00
1.140000E+03	1.028	-0.028	5.418227E-02	3.333333E-01	-1.706354E+00
1.150000E+03	1.033	-0.033	5.554314E-02	3.333333E-01	-1.725275E+00
1.160000E+03	1.038	-0.038	5.691756E-02	3.333333E-01	-1.743868E+00
1.170000E+03	1.043	-0.043	5.830566E-02	3.333333E-01	-1.762134E+00
1.180000E+03	1.048	-0.048	5.970756E-02	3.333333E-01	-1.780075E+00
1.190000E+03	1.054	-0.054	6.112340E-02	3.333333E-01	-1.797692E+00
1.200000E+03	1.059	-0.059	6.255334E-02	3.333333E-01	-1.814987E+00

\*\*\* Buffer savend on file

c:\jenkins\WORKSP~1\THERMO~1\examples\tcex42\TCEX42~2.POL

POLY\_3:

POLY\_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-d-a x w(\*,c)

... the command in full is SET\_DIAGRAM\_AXIS

COLUMN NUMBER /\*/: \*

POST: s-d-a y t-k

... the command in full is SET\_DIAGRAM\_AXIS

POST: s-a-text x n MASS U-FRACTION, C

... the command in full is SET\_AXIS\_TEXT\_STATUS

POST: set-tie 5

... the command in full is SET\_TIELINE\_STATUS

POST: set-tit example 42d

... the command in full is SET\_TITLE

POST: app-e n

... the command in full is APPEND\_EXPERIMENTAL\_DATA

POST:

POST: plot

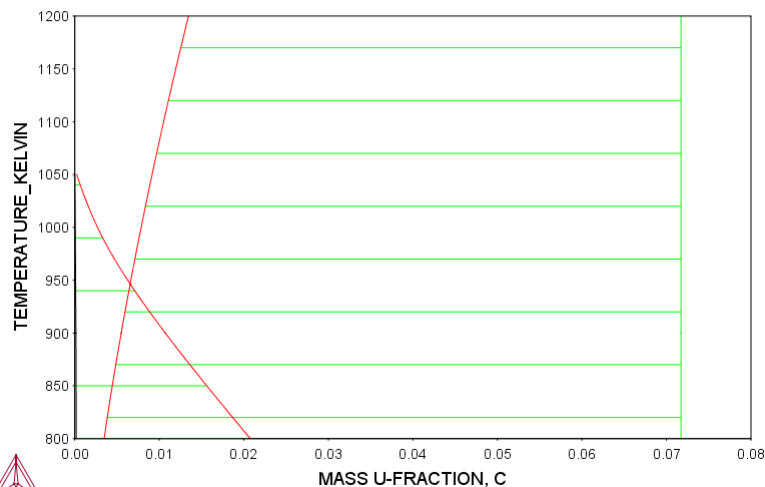
... the command in full is PLOT DIAGRAM

example 42d

2016.05.16.14.33.13

TCFE7: C, FE, MN

P=1E5, N=1., W(C)=1E-2, W(MN)=2.5E-2



POST:

POST:Hit RETURN to continue

POST:

POST: app-e y tcex42

... the command in full is APPEND\_EXPERIMENTAL\_DATA

PROLOGUE NUMBER: /0/: 0

DATASET NUMBER(s): /-1/: 1

POST: s-s x n 0 0.02

... the command in full is SET\_SCALING\_STATUS

POST: set-title example 42e

POST:

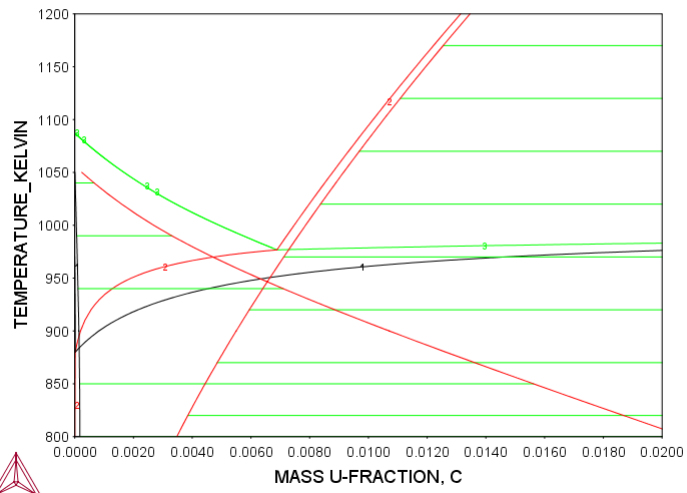
POST: plot

... the command in full is PLOT\_DIAGRAM

# example 42e

2016.05.16.14.33.14  
TCFE7: C, FE, MN  
P=1E5, N=1., W(C)=1E-2, W(MN)=2.5E-2

1\*FCC\_A1  
2\*CEMENTITE  
3\*BCC\_A2



POST:  
POST: set-inter  
... the command in full is SET\_INTERACTIVE\_MODE  
POST:

## About

```

SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex43\tcex43.TCM" set-echo
SYS: @@
SYS: @@
SYS: @@ Paraequilibrium calculation - Formation of Para-pearlite - Isothermal
SYS: @@
SYS: @@ Fe-Mn-C system at 700 C
SYS: @@
SYS: set-log ex43,,,
SYS: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3: d-mater
... the command in full is DEFINE_MATERIAL
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
L12_FCC          B2_BCC          B2_VACANCY
HIGH_SIGMA      DICTRA_FCC_A1   REJECTED
Database /TCFE8/: tcfe7
Current database: Steels/Fe-Alloys v7.0

VA DEFINED
L12_FCC          B2_BCC          B2_VACANCY
HIGH_SIGMA      DICTRA_FCC_A1   REJECTED
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/: Y
1st alloying element: c 0.1
2nd alloying element: mn 2
Next alloying element:
Temperature (C) /1000/: 700
VA DEFINED
L12_FCC          B2_BCC          B2_VACANCY
HIGH_SIGMA      DICTRA_FCC_A1   REJECTED
REINITIATING GES5 .....
... the command in full is DEFINE_ELEMENTS
FE DEFINED
... the command in full is DEFINE_ELEMENTS
C DEFINED
... the command in full is DEFINE_ELEMENTS
MN DEFINED

This database has following phases for the defined system

GAS:G            LIQUID:L            BCC_A2
FCC_A1           HCP_A3            DIAMOND_FCC_A4
GRAPHITE         CEMENTITE         M23C6
M7C3            M5C2              KSI_CARBIIDE
A1_KAPPA        KAPPA            FE4N_LP1
FECN_CHI        LAVES_PHASE_C14   G_PHASE

Reject phase(s) /NONE/: graphite m5c2
GRAPHITE         M5C2   REJECTED
Reject phase(s) /NONE/: NONE
Restore phase(s) : /NONE/: NONE

.....

The following phases are retained in this system:

GAS:G            LIQUID:L            BCC_A2
FCC_A1           HCP_A3            DIAMOND_FCC_A4
CEMENTITE        M23C6            M7C3
KSI_CARBIIDE     A1_KAPPA         KAPPA
FE4N_LP1         FECN_CHI        LAVES_PHASE_C14
G_PHASE

.....

OK? /Y/: Y
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
-FE'
'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
'W. Huang, Calphad, 13 (1989), 243-252; TRITA-MAC 388 (rev 1989); FE-MN'
'P. Franke, estimated parameter within SGTE, 2008; Fe-Mn-C'
'B. Uhrenius (1993-1994), International journal of refractory metals and
hard mater, Vol. 12, pp. 121-127; Molar volumes'
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
Molar volumes'
'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
'W. Huang, Metall. Trans. A, 21A (1990), 2115-2123; TRITA-MAC 411 (Rev
1989); C-FE-MN'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
'P. Villars and L.D. Calvert (1985). Pearsons handbook of crystallographic
data for intermetallic phases. Metals park, Ohio. American Society for
Metals; Molar volumes'
'J-O. Andersson, Metall. Trans. A, 19A (1988), 627-636 TRITA 0207 (1986);
C-CR-FE'
'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'
'J-O. Andersson, Calphad, 12 (1988), 9-23; TRITA 0321 (1986); C-FE-MO'
'D. Connetable, J. Lacaze, P. Maugis and B. Sundman; Calphad, Vol. 32
(2008), pp. 361-370; Al-C-Fe'
'Thermo-Calc Software (2008): Volume data updated for TCFE6 database (TCFE

```

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v6, April, 2008).'
'H. Du and M. Hillert, TRITA-MAC 435 (1990); C-Fe-N'
'Estimated parameter for solubility of C in Fe4N, 1999'
'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equil., 19 (1998),
  441-448; Fe-Ti'
'N. Saunders, COST 507 Report (1998); Mn-Ti'
'A. Markstrom, Thermo-Calc software AB, 2011'
-OK-
Should any phase have a miscibility gap check? /N/: N
Using global minimization procedure
Calculated          13031 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution      1 s, total time      1 s
POLY_3: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
Output from POLY-3, equilibrium =      1, label A0  , database: TCFe7

Conditions:
T=973.15, W(C)=1E-3, W(MN)=2E-2, P=1E5, N=1
DEGREES OF FREEDOM 0

Temperature      973.15 K (   700.00 C), Pressure  1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams  5.56256E+01
Total Gibbs energy -4.11739E+04, Enthalpy  2.46047E+04, Volume  7.28123E-06

Component      Moles      W-Fraction Activity Potential Ref.stat
C               4.6312E-03  1.0000E-03 1.2824E-01 -1.6618E+04 SER
FE              9.7512E-01  9.7900E-01 6.6199E-03 -4.0599E+04 SER
MN              2.0250E-02  2.0000E-02 1.0082E-04 -7.4457E+04 SER

BCC_A2          Status ENTERED      Driving force  0.0000E+00
Moles 7.8346E-01, Mass 4.3734E+01, Volume fraction 7.8722E-01 Mass fractions:
FE 9.86998E-01 MN 1.29345E-02 C 6.74179E-05

FCC_A1          Status ENTERED      Driving force  0.0000E+00
Moles 2.1654E-01, Mass 1.1892E+01, Volume fraction 2.1278E-01 Mass fractions:
FE 9.49585E-01 MN 4.59849E-02 C 4.42980E-03
POLY_3: @@
POLY_3: @@ change the status of component C to SPECIAL and work with u-fractions
POLY_3: @@
POLY_3: c-s comp c
... the command in full is CHANGE_STATUS
Status: /ENTERED/: spe
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated          13031 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution      0 s, total time      0 s
POLY_3: s-a-v 1 w(c) 0 0.08
... the command in full is SET_AXIS_VARIABLE
Increment /.002/: 2.5E-04
POLY_3: s-a-v 2 w(mn) 0 0.1
... the command in full is SET_AXIS_VARIABLE
Increment /.0025/: .0025
POLY_3: l-a-v
... the command in full is LIST_AXIS_VARIABLE
Axis No 1: W(C)          Min: 0          Max: 8E-2          Inc: 2.5E-4
Axis No 2: W(MN)         Min: 0          Max: 0.1          Inc: 2.5E-3
POLY_3: sa tcex43a y
... the command in full is SAVE_WORKSPACES
POLY_3: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28
Generating start point 29
Generating start point 30
Working hard

```

```

Generating start point 31
Generating start point 32

Phase region boundary 1 at: 3.082E-02 1.466E-02
  BCC_A2
  ** CEMENTITE
Calculated 18 equilibria

Phase region boundary 2 at: 3.082E-02 1.466E-02
  BCC_A2
  ** CEMENTITE
Calculated. 11 equilibria

Phase region boundary 3 at: 3.082E-02 3.943E-02
  BCC_A2
  ** CEMENTITE
  ** FCC_A1

Phase region boundary 4 at: 3.392E-03 1.781E-02
  BCC_A2
  ** FCC_A1
Calculated 34 equilibria

Phase region boundary 5 at: 3.511E-02 5.220E-02
  CEMENTITE
  ** FCC_A1
Calculated.. 48 equilibria
Terminating at axis limit.

Phase region boundary 6 at: 3.082E-02 3.943E-02
  BCC_A2
  ** CEMENTITE
Calculated 27 equilibria

Phase region boundary 7 at: 3.082E-02 1.466E-02
  BCC_A2
  ** CEMENTITE
Calculated 18 equilibria

Phase region boundary 8 at: 3.082E-02 1.466E-02
  BCC_A2
  ** CEMENTITE
Calculated. 11 equilibria
Terminating at known equilibrium

Phase region boundary 9 at: 3.082E-02 2.813E-03
  BCC_A2
  ** CEMENTITE
Calculated 10 equilibria

Phase region boundary 10 at: 3.082E-02 2.813E-03
  BCC_A2
  ** CEMENTITE
Calculated. 16 equilibria
Terminating at known equilibrium

Phase region boundary 11 at: 3.082E-02 1.549E-03
  BCC_A2
  ** CEMENTITE
Calculated 13 equilibria

Phase region boundary 12 at: 3.082E-02 1.549E-03
  BCC_A2
  ** CEMENTITE
Calculated. 17 equilibria
Terminating at known equilibrium

Phase region boundary 13 at: 3.585E-01 2.500E-03
  CEMENTITE
  ** DIAMOND_FCC_A4
Calculated 22 equilibria

Phase region boundary 14 at: 3.585E-01 2.500E-03
  CEMENTITE
  ** DIAMOND_FCC_A4
Calculated. 133 equilibria

Phase region boundary 15 at: 3.604E-01 3.323E-01
  CEMENTITE
  ** DIAMOND_FCC_A4
  ** M7C3

Phase region boundary 16 at: 8.213E-02 4.124E-01
  CEMENTITE
  ** M7C3

Phase region boundary 17 at: 4.027E-01 4.984E-01
  DIAMOND_FCC_A4
  ** M7C3

Phase region boundary 18 at: 3.604E-01 3.323E-01
  CEMENTITE
  ** DIAMOND_FCC_A4
Calculated 142 equilibria

Phase region boundary 19 at: 3.585E-01 2.500E-03
  CEMENTITE
  ** DIAMOND_FCC_A4
Calculated 22 equilibria

Phase region boundary 20 at: 3.585E-01 2.500E-03
  CEMENTITE
  ** DIAMOND_FCC_A4
Calculated. 133 equilibria
Terminating at known equilibrium

Phase region boundary 21 at: 4.549E-04 4.437E-02
  BCC_A2
  ** FCC_A1
Calculated. 19 equilibria
Terminating at known equilibrium

Phase region boundary 22 at: 4.549E-04 4.437E-02
  BCC_A2
  ** FCC_A1
Calculated 13 equilibria

```

Phase region boundary 23 at: 3.587E-01 3.417E-02  
CEMENTITE  
\*\* DIAMOND\_FCC\_A4  
Calculated 26 equilibria

Phase region boundary 24 at: 3.587E-01 3.417E-02  
CEMENTITE  
\*\* DIAMOND\_FCC\_A4  
Calculated. 121 equilibria  
Terminating at known equilibrium

Phase region boundary 25 at: 1.375E-04 4.677E-02  
\*\* BCC\_A2  
FCC\_A1  
Calculated. 19 equilibria  
Terminating at known equilibrium

Phase region boundary 26 at: 1.375E-04 4.677E-02  
\*\* BCC\_A2  
FCC\_A1  
Calculated 19 equilibria

Phase region boundary 27 at: 3.588E-01 6.583E-02  
CEMENTITE  
\*\* DIAMOND\_FCC\_A4  
Calculated 38 equilibria

Phase region boundary 28 at: 3.588E-01 6.583E-02  
CEMENTITE  
\*\* DIAMOND\_FCC\_A4  
Calculated. 108 equilibria  
Terminating at known equilibrium

Phase region boundary 29 at: 3.488E-02 1.652E-01  
\*\* CEMENTITE  
FCC\_A1  
Calculated. 47 equilibria  
Terminating at known equilibrium

Phase region boundary 30 at: 3.488E-02 1.652E-01  
\*\* CEMENTITE  
FCC\_A1  
Calculated.. 3 equilibria  
Terminating at axis limit.

Phase region boundary 31 at: 3.488E-02 1.677E-01  
\*\* CEMENTITE  
FCC\_A1  
Calculated. 48 equilibria  
Terminating at known equilibrium

Phase region boundary 32 at: 1.264E-04 4.685E-02  
\*\* BCC\_A2  
FCC\_A1  
Calculated 9 equilibria

Phase region boundary 33 at: 1.264E-04 4.685E-02  
\*\* BCC\_A2  
FCC\_A1  
Calculated. 15 equilibria  
Terminating at known equilibrium

Phase region boundary 34 at: 3.498E-02 1.113E-01  
\*\* CEMENTITE  
FCC\_A1  
Calculated. 25 equilibria  
Terminating at known equilibrium

Phase region boundary 35 at: 3.498E-02 1.113E-01  
\*\* CEMENTITE  
FCC\_A1  
Calculated.. 25 equilibria  
Terminating at axis limit.

Phase region boundary 36 at: 3.488E-02 1.688E-01  
\*\* CEMENTITE  
FCC\_A1  
Calculated. 48 equilibria  
Terminating at known equilibrium

Phase region boundary 37 at: 3.506E-02 7.604E-02  
\*\* CEMENTITE  
FCC\_A1  
Calculated. 11 equilibria  
Terminating at known equilibrium

Phase region boundary 38 at: 3.506E-02 7.604E-02  
\*\* CEMENTITE  
FCC\_A1  
Calculated.. 39 equilibria  
Terminating at axis limit.

Phase region boundary 39 at: 3.488E-02 1.685E-01  
\*\* CEMENTITE  
FCC\_A1  
Calculated. 48 equilibria  
Terminating at known equilibrium

Phase region boundary 40 at: 3.590E-01 9.750E-02  
CEMENTITE  
\*\* DIAMOND\_FCC\_A4  
Calculated 42 equilibria

Phase region boundary 41 at: 3.590E-01 9.750E-02  
CEMENTITE  
\*\* DIAMOND\_FCC\_A4  
Calculated. 95 equilibria  
Terminating at known equilibrium

Phase region boundary 42 at: 3.590E-01 9.750E-02  
CEMENTITE  
\*\* DIAMOND\_FCC\_A4  
Calculated 42 equilibria

Phase region boundary 43 at: 3.590E-01 9.750E-02

```

CEMENTITE
** DIAMOND_FCC_A4
Calculated.          95 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex43\tcex
43a.POLY3
CPU time for mapping          4 seconds

```

```

POLY_3:
POLY_3: post

```

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

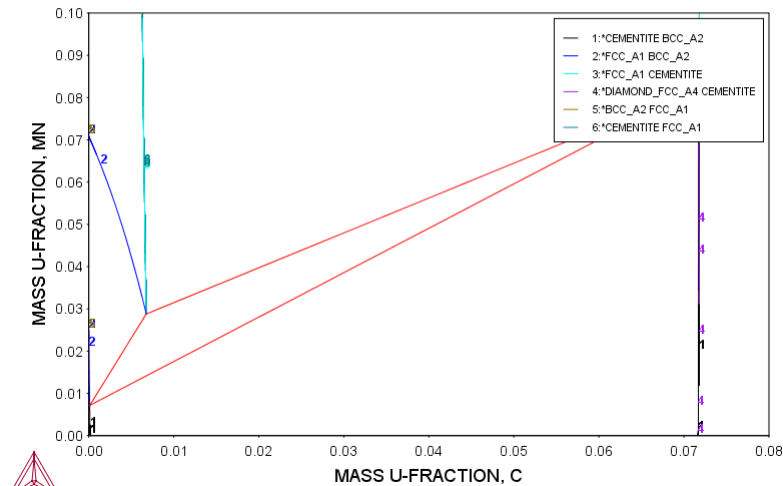
```

POST: s-lab e
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-title example 43a
POST: s-ax-text x N MASS U-FRACTION, C
... the command in full is SET_AXIS_TEXT_STATUS
POST: s-ax-text y N MASS U-FRACTION, MN
... the command in full is SET_AXIS_TEXT_STATUS
POST: plot
... the command in full is PLOT DIAGRAM

```

example 43a

2016.05.16.14.35.38  
TCFE7: C, FE, MN  
T=973.15, P=1E5, N=1



```

POST:
POST:Hit RETURN to continue
POST:
POST: make tcex43 y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST: b
... the command in full is BACK
POLY_3: read tcex43a
... the command in full is READ_WORKSPACES
POLY_3: s-a-v 1 w(mn) 0 0.1
... the command in full is SET_AXIS_VARIABLE
Increment /.0025/ : .0025
POLY_3: s-a-v 2 none
... the command in full is SET_AXIS_VARIABLE
POLY_3: sa tcex43b y
... the command in full is SAVE_WORKSPACES
POLY_3: step
... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: para

```

This command calculates a paraequilibrium between two phases.  
You must calculate an equilibrium with the overall composition first.

```

Name of first phase: fcc_a1
Name of second phase: bcc_a2
Fast diffusing component: /C/: C
Fast diffusing component: /NONE/:

```

Output during stepping is:  
axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,  
and LNACR value(s) of interstitial(s)

Phase Region from 0.200000E-01 for:					
BCC_A2 FCC_A1					
2.000000E-02	0.165	0.835	2.571485E-02	4.910396E-04	-1.652126E+00
1.750000E-02	0.148	0.852	2.818000E-02	5.485823E-04	-1.524121E+00
1.500000E-02	0.135	0.865	3.063880E-02	6.079802E-04	-1.404111E+00
1.250000E-02	0.123	0.877	3.309067E-02	6.692476E-04	-1.290883E+00
1.000000E-02	0.113	0.887	3.553566E-02	7.324129E-04	-1.183465E+00
7.500000E-03	0.104	0.896	3.797362E-02	7.974991E-04	-1.081091E+00
5.000000E-03	0.096	0.904	4.040445E-02	8.645295E-04	-9.831360E-01
2.500000E-03	0.089	0.911	4.282805E-02	9.335273E-04	-8.890905E-01
2.500000E-09	0.082	0.918	4.524437E-02	1.004515E-03	-7.985285E-01

Phase Region from 0.200000E-01 for:					
BCC_A2 FCC_A1					
2.000000E-02	0.165	0.835	2.571485E-02	4.910396E-04	-1.652126E+00
2.250000E-02	0.185	0.815	2.324342E-02	4.353248E-04	-1.789740E+00
2.500000E-02	0.209	0.791	2.076601E-02	3.814145E-04	-1.939115E+00
2.750000E-02	0.241	0.759	1.828295E-02	3.292857E-04	-2.103233E+00
3.000000E-02	0.282	0.718	1.579466E-02	2.789151E-04	-2.286396E+00
3.250000E-02	0.338	0.662	1.330158E-02	2.302795E-04	-2.495141E+00
3.500000E-02	0.420	0.580	1.080428E-02	1.833559E-04	-2.740125E+00
3.750000E-02	0.552	0.448	8.303377E-03	1.381213E-04	-3.040528E+00
4.000000E-02	0.798	0.202	5.799614E-03	9.455272E-05	-3.436595E+00
4.250000E-02	1.418	-0.418	3.293836E-03	5.262739E-05	-4.039594E+00

```
4.500000E-02 5.984 -4.984 7.870255E-04 1.232263E-05 -5.508458E+00
*** Buffer savend on file
c:\jenkins\WORKSP~1\THERMO~1\examples\tcex43\TCEX43~2.POL
```

```
*** ERROR      3 IN NS01AD
*** Numerical error
POLY_3: po
... the command in full is POST

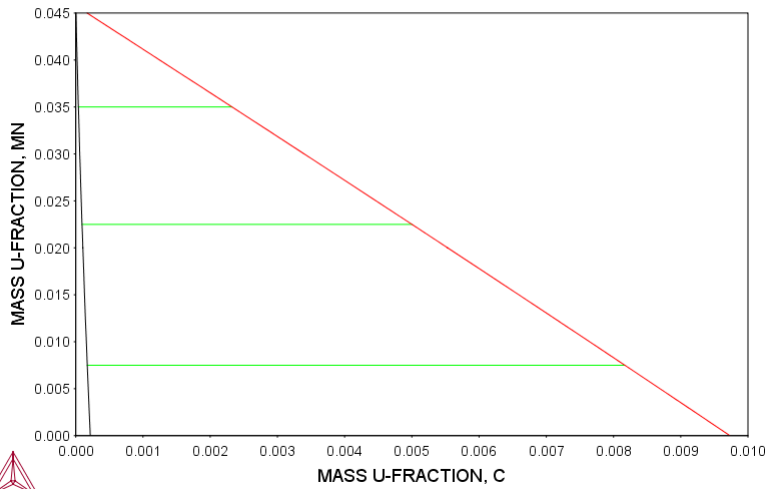
POLY-3 POSTPROCESSOR VERSION 3.2
```

Setting automatic diagram axes

```
POST: s-d-a x w(*,c)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: s-d-a y w(*,mn)
... the command in full is SET_DIAGRAM_AXIS
COLUMN NUMBER /*/: *
POST: set-tie 5
... the command in full is SET_TIELINE_STATUS
POST: set-title example 43b
POST: s-ax-text x N MASS U-FRACTION, C
... the command in full is SET_AXIS_TEXT_STATUS
POST: s-ax-text y N MASS U-FRACTION, MN
... the command in full is SET_AXIS_TEXT_STATUS
POST:
POST: plot
... the command in full is PLOT DIAGRAM
```

example 43b

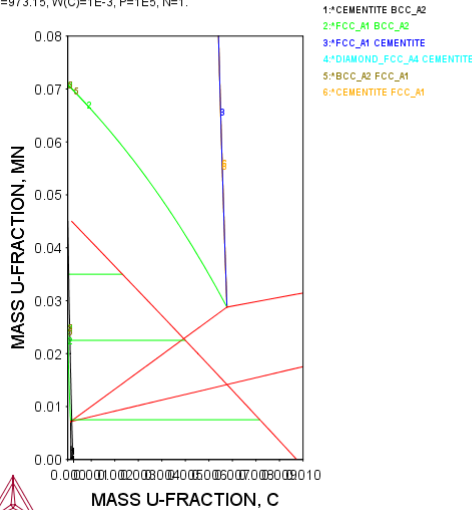
2016.05.16.14.35.40  
TCFE7: C, FE, MN  
T=973.15, W(C)=1E-3, P=1E5, N=1.



```
POST:
POST:Hit RETURN to continue
POST:
POST: app y tcex43
... the command in full is APPEND_EXPERIMENTAL_DATA
PROLOGUE NUMBER: /0/: 0
DATASET NUMBER(s): /-1/: 1
POST: s-s x n 0 0.01
... the command in full is SET_SCALING_STATUS
POST: s-s y n 0 0.08
... the command in full is SET_SCALING_STATUS
POST: set-title example 43c
POST:
POST: plot
... the command in full is PLOT DIAGRAM
```

example 43c

2016.05.16.14.35.40  
TCFE7: C, FE, MN  
T=973.15, W(C)=1E-3, P=1E5, N=1.



```
POST:
POST:Hit RETURN to continue
POST:
```



```

POST: b
... the command in full is BACK
POLY_3: read tcex43b
... the command in full is READ_WORKSPACES
POLY_3: l-c
... the command in full is LIST_CONDITIONS
T=973.15, W(C)=1E-3, W(MN)=2E-2, P=1E5, N=1
DEGREES OF FREEDOM 0
POLY_3: s-c w(c)=0.008 w(mn)=0.07
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 13031 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY_3: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
Output from POLY-3, equilibrium = 1, label A0 , database: TCFE7

Conditions:
T=973.15, W(C)=8E-3, W(MN)=7E-2, P=1E5, N=1
DEGREES OF FREEDOM 0

Temperature 973.15 K ( 700.00 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 5.42144E+01
Total Gibbs energy -4.19857E+04, Enthalpy 2.75863E+04, Volume 7.10872E-06

Component      Moles      W-Fraction  Activity   Potential  Ref.stat
C               3.5823E-02  8.0000E-03  1.8345E-01 -1.3721E+04 SER
FE              8.9565E-01  9.3000E-01  6.4227E-03 -4.0844E+04 SER
MN              6.8530E-02  7.0000E-02  1.4208E-04 -7.1681E+04 SER

FCC_A1          Status ENTERED   Driving force 0.0000E+00
Moles 9.7022E-01, Mass 5.2881E+01, Volume fraction 9.7477E-01 Mass fractions:
FE 9.26648E-01 MN 6.69068E-02 C 6.44559E-03

CEMENTITE       Status ENTERED   Driving force 0.0000E+00
Moles 2.9780E-02, Mass 1.3330E+00, Volume fraction 2.5229E-02 Mass fractions:
FE 7.62802E-01 MN 1.70116E-01 C 6.70826E-02
POLY_3: advanced
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: para

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc_al
Name of second phase: cementite
Fast diffusing component: /C/: C
Fast diffusing component: /NONE/:
NP(FCC A1) = 0.9928 with U-fractions C = 3.50068E-02
NP(CEMENTITE) = 0.0072 with U-fractions C = 3.33333E-01
All other compositions the same in both phases
Note: LIST-EQUILIBRIUM is not relevant
POLY_3: step
... the command in full is STEP_WITH_OPTIONS
Option? /NORMAL/: para

This command calculates a paraequilibrium between two phases.
You must calculate an equilibrium with the overall composition first.
Name of first phase: fcc_al
Name of second phase: cementite
Fast diffusing component: /C/: C
Fast diffusing component: /NONE/:
Output during stepping is:
axis value, phase amounts, u-fractions of interstitial(s) in phase 1 and 2,
and LNACR value(s) of interstitial(s)

Phase Region from 0.700000E-01 for:
CEMENTITE
FCC_A1
7.000000E-02 0.993 0.007 3.500676E-02 3.333333E-01 -1.512238E+00
6.750000E-02 0.993 0.007 3.491610E-02 3.333333E-01 -1.502576E+00
6.500000E-02 0.992 0.008 3.482586E-02 3.333333E-01 -1.492928E+00
6.250000E-02 0.992 0.008 3.473603E-02 3.333333E-01 -1.483293E+00
6.000000E-02 0.992 0.008 3.464662E-02 3.333333E-01 -1.473672E+00
5.750000E-02 0.991 0.009 3.455761E-02 3.333333E-01 -1.464066E+00
5.500000E-02 0.991 0.009 3.446901E-02 3.333333E-01 -1.454473E+00
5.250000E-02 0.991 0.009 3.438081E-02 3.333333E-01 -1.444894E+00
5.000000E-02 0.990 0.010 3.429302E-02 3.333333E-01 -1.435329E+00
4.750000E-02 0.990 0.010 3.420563E-02 3.333333E-01 -1.425778E+00
4.500000E-02 0.990 0.010 3.411864E-02 3.333333E-01 -1.416242E+00
4.250000E-02 0.990 0.010 3.403205E-02 3.333333E-01 -1.406719E+00
4.000000E-02 0.989 0.011 3.394585E-02 3.333333E-01 -1.397211E+00
3.750000E-02 0.989 0.011 3.386005E-02 3.333333E-01 -1.387717E+00
3.500000E-02 0.989 0.011 3.377464E-02 3.333333E-01 -1.378237E+00
3.250000E-02 0.988 0.012 3.368963E-02 3.333333E-01 -1.368772E+00
3.000000E-02 0.988 0.012 3.360500E-02 3.333333E-01 -1.359321E+00
2.750000E-02 0.988 0.012 3.352076E-02 3.333333E-01 -1.349884E+00
2.500000E-02 0.988 0.012 3.343690E-02 3.333333E-01 -1.340462E+00
2.250000E-02 0.987 0.013 3.335343E-02 3.333333E-01 -1.331054E+00
2.000000E-02 0.987 0.013 3.327034E-02 3.333333E-01 -1.321660E+00
1.750000E-02 0.987 0.013 3.318763E-02 3.333333E-01 -1.312282E+00
1.500000E-02 0.987 0.013 3.310530E-02 3.333333E-01 -1.302918E+00
1.250000E-02 0.986 0.014 3.302335E-02 3.333333E-01 -1.293568E+00
1.000000E-02 0.986 0.014 3.294177E-02 3.333333E-01 -1.284233E+00
7.500000E-03 0.986 0.014 3.286057E-02 3.333333E-01 -1.274913E+00
5.000000E-03 0.985 0.015 3.277974E-02 3.333333E-01 -1.265607E+00
2.500000E-03 0.985 0.015 3.269928E-02 3.333333E-01 -1.256316E+00
2.500000E-09 0.985 0.015 3.261919E-02 3.333333E-01 -1.247040E+00

Phase Region from 0.700000E-01 for:
CEMENTITE
FCC_A1
7.000000E-02 0.993 0.007 3.500676E-02 3.333333E-01 -1.512238E+00
7.250000E-02 0.993 0.007 3.509783E-02 3.333333E-01 -1.521914E+00
7.500000E-02 0.993 0.007 3.518931E-02 3.333333E-01 -1.531604E+00
7.750000E-02 0.994 0.006 3.528122E-02 3.333333E-01 -1.541307E+00
8.000000E-02 0.994 0.006 3.537355E-02 3.333333E-01 -1.551024E+00
8.250000E-02 0.994 0.006 3.546630E-02 3.333333E-01 -1.560755E+00
8.500000E-02 0.995 0.005 3.555948E-02 3.333333E-01 -1.570499E+00
8.750000E-02 0.995 0.005 3.565309E-02 3.333333E-01 -1.580257E+00
9.000000E-02 0.995 0.005 3.574712E-02 3.333333E-01 -1.590028E+00

```

```

9.250000E-02  0.996  0.004  3.584159E-02  3.333333E-01  -1.599812E+00
9.500000E-02  0.996  0.004  3.593649E-02  3.333333E-01  -1.609610E+00
9.750000E-02  0.996  0.004  3.603182E-02  3.333333E-01  -1.619421E+00
1.000000E-01  0.997  0.003  3.612760E-02  3.333333E-01  -1.629246E+00

```

\*\*\* Buffer savend on file

c:\jenkins\WORKSP~1\THERMO~1\examples\tcex43\TCEX43~2.POL

POLY\_3: po

... the command in full is POST

POLY-3 POSTPROCESSOR VERSION 3.2

POST: s-d-a x w(\*,c)

... the command in full is SET\_DIAGRAM\_AXIS

COLUMN NUMBER /\*/: \*

POST: s-d-a y w(\*,mn)

... the command in full is SET\_DIAGRAM\_AXIS

COLUMN NUMBER /\*/: \*

POST: set-tie 5

... the command in full is SET\_TIELINE\_STATUS

POST: set-title example 43d

POST: s-ax-text x N MASS U-FRACTION, C

... the command in full is SET\_AXIS\_TEXT\_STATUS

POST: s-ax-text y N MASS U-FRACTION, MN

... the command in full is SET\_AXIS\_TEXT\_STATUS

POST: app-e n

... the command in full is APPEND\_EXPERIMENTAL\_DATA

POST:

POST: plot

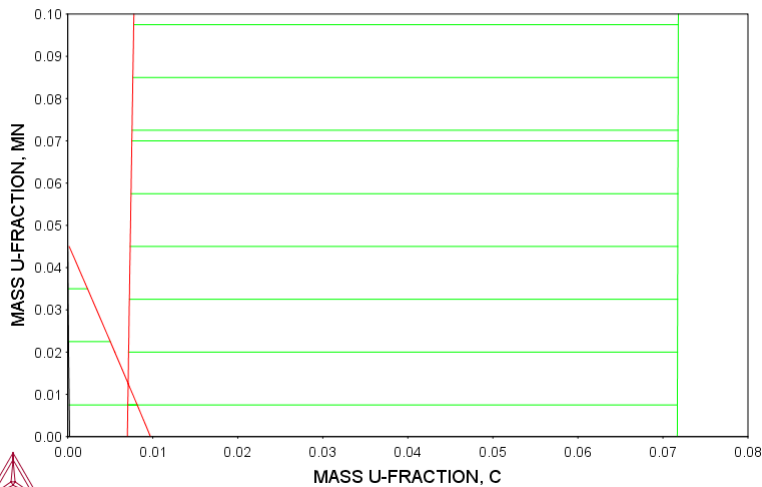
... the command in full is PLOT DIAGRAM

example 43d

2016.05.16.14.35.43

TCFE7: C, FE, MN

T=973.15, W(C)=8E-3, P=1E5, N=1.



POST:

POST:

POST: Hit RETURN to continue

POST:

POST: s-s x n 0 0.01

... the command in full is SET\_SCALING\_STATUS

POST: s-s y n 0 0.10

... the command in full is SET\_SCALING\_STATUS

POST: app-e y tcex43

... the command in full is APPEND\_EXPERIMENTAL\_DATA

PROLOGUE NUMBER: /0/: 0

DATASET NUMBER(s): /-1/: 1

POST: set-title example 43e

POST:

POST: plot

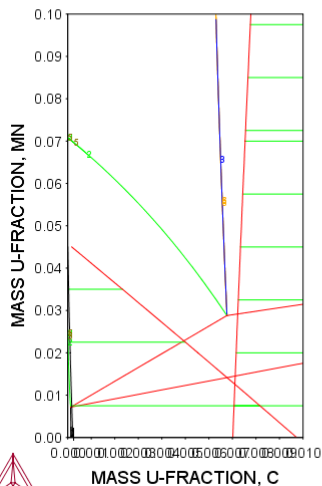
... the command in full is PLOT DIAGRAM

example 43e

2016.05.16.14.35.44

TCFE7: C, FE, MN

T=973.15, W(C)=8E-3, P=1E5, N=1.



1\*CEMENTITE BCC\_A2  
2\*FCC\_A1 BCC\_A2  
3\*FCC\_A1 CEMENTITE  
4\*DIAMOND\_FCC\_A4 CEMENTITE  
5\*BCC\_A2 FCC\_A1  
6\*CEMENTITE FCC\_A1

POST:

POST: set-inter

... the command in full is SET\_INTERACTIVE\_MODE



```

AboutMACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex44\tcex44.TCM" set-echo
SYS: @@
SYS: @@ Exploring the usage of variables and functions. Proof strength for an austenitic stainless steel at elevated temperatures.
SYS: @@
SYS: @@
SYS: @@ Exploring the usage of variables and functions in order to predict
SYS: @@ properties e.g. Proof strength for an austenitic stainless
SYS: @@ steel (20-550C)
SYS:
SYS: go da
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
L12_FCC                B2_BCC                B2_VACANCY
HIGH_SIGMA            DICTRA_FCC_A1    REJECTED
TDB_TCFE8: sw tcfe7
Current database: Steels/Fe-Alloys v7.0

VA DEFINED
L12_FCC                B2_BCC                B2_VACANCY
HIGH_SIGMA            DICTRA_FCC_A1    REJECTED
TDB_TCFE7: def-sys
ELEMENTS: fe c si mn cr ni mo cu n
FE                    C                    SI
MN                    CR                    NI
MO                    CU                    N
      DEFINED
TDB_TCFE7: get
REINITIATING GES5 .....
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

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-OK-

**TDB\_TCFe7:**

**TDB\_TCFe7:** go p-3

POLY version 3.32  
**POLY\_3:**  
**POLY\_3:** s-c p=1e5,n=1,t=1353  
**POLY\_3:** s-c w(c)=0.0009,w(n)=0.0007,w(cr)=.246,w(ni)=0.2,w(mn)=0.013  
**POLY\_3:** s-c w(si)=0.013,w(cu)=0.0024,w(mo)=0.003  
**POLY\_3:** l-c  
P=1E5, N=1, T=1353, W(C)=9E-4, W(N)=7E-4, W(CR)=0.246, W(NI)=0.2,  
W(MN)=1.3E-2, W(SI)=1.3E-2, W(CU)=2.4E-3, W(MO)=3E-3  
DEGREES OF FREEDOM 0  
**POLY\_3:** c-e  
Using global minimization procedure  
Calculated 34286 grid points in 1 s  
Found the set of lowest grid points in 0 s  
Calculated POLY solution 0 s, total time 1 s  
**POLY\_3:** l-e  
**OUTPUT TO SCREEN OR FILE /SCREEN/:**  
**Options /VWCS/:** VWCS  
Output from POLY-3, equilibrium = 1, label A0 , database: TCFe7  
  
Conditions:  
P=1E5, N=1, T=1353, W(C)=9E-4, W(N)=7E-4, W(CR)=0.246, W(NI)=0.2,  
W(MN)=1.3E-2, W(SI)=1.3E-2, W(CU)=2.4E-3, W(MO)=3E-3  
DEGREES OF FREEDOM 0  
  
Temperature 1353.00 K ( 1079.85 C), Pressure 1.000000E+05  
Number of moles of components 1.00000E+00, Mass in grams 5.44622E+01  
Total Gibbs energy -8.11772E+04, Enthalpy 3.59088E+04, Volume 7.33318E-06  
  

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
C	4.0809E-03	9.0000E-04	1.3125E-03	-7.4650E+04	SER
CR	2.5767E-01	2.4600E-01	2.7776E-03	-6.6217E+04	SER
CU	2.0569E-03	2.4000E-03	8.2084E-05	-1.0583E+05	SER
FE	5.0808E-01	5.2100E-01	1.1351E-03	-7.6283E+04	SER

```

MN          1.2887E-02  1.3000E-02  6.4085E-06 -1.3452E+05 SER
MO          1.7030E-03  3.0000E-03  6.2271E-05 -1.0894E+05 SER
N           2.7217E-03  7.0000E-04  1.5560E-07 -1.7635E+05 SER
NI          1.8559E-01  2.0000E-01  2.2145E-04 -9.4668E+04 SER
SI          2.5209E-02  1.3000E-02  3.5318E-08 -1.9303E+05 SER

FCC_A1          Status ENTERED      Driving force  0.0000E+00
Moles 9.9426E-01, Mass 5.4205E+01, Volume fraction 9.9495E-01  Mass fractions:
FE 5.22729E-01  SI 1.30618E-02  CU 2.41140E-03
CR 2.43674E-01  MN 1.30378E-02  N  7.03326E-04
NI 2.00856E-01  MO 2.88542E-03  C  6.41161E-04

M23C6          Status ENTERED      Driving force  0.0000E+00
Moles 5.7392E-03, Mass 2.5758E-01, Volume fraction 5.0456E-03  Mass fractions:
CR 7.35501E-01  MO 2.71117E-02  N  0.00000E+00
FE 1.57176E-01  NI 1.97963E-02  CU 0.00000E+00
C  5.53701E-02  MN 5.04497E-03  SI 0.00000E+00

POLY_3:
POLY_3: @@ Define some variables
POLY_3: enter-symb
Constant, variable, function or table? /FUNCTION/: variable
Name: cc
Function: 100*w(fcc_a1,c)
&
POLY_3: ent var csi=100*w(fcc_a1,si);
POLY_3: ent var cmn=100*w(fcc_a1,mn);
POLY_3: ent var ccr=100*w(fcc_a1,cr);
POLY_3: ent var cni=100*w(fcc_a1,ni);
POLY_3: ent var cmo=100*w(fcc_a1,mo);
POLY_3: ent var ccu=100*w(fcc_a1,cu);
POLY_3: ent var cn=100*w(fcc_a1,n);
POLY_3: ent var cfe=100*w(fcc_a1,fe);
POLY_3: ent var cm23=100*bpw(m23c6);
POLY_3:
POLY_3: li-sy
DEFINED FUNCTIONS AND VARIABLES%
CC%=100*W(FCC_A1,C)
CSI%=100*W(FCC_A1,SI)
CMN%=100*W(FCC_A1,MN)
CCR%=100*W(FCC_A1,CR)
CNI%=100*W(FCC_A1,NI)
CMO%=100*W(FCC_A1,MO)
CCU%=100*W(FCC_A1,CU)
CN%=100*W(FCC_A1,N)
CFE%=100*W(FCC_A1,FE)
CM23%=100*BPW(M23C6)
POLY_3:
POLY_3: eval
Name(s): *
CC=6.4116133E-2
CSI=1.3061775
CMN=1.3037802
CCR=24.367392
CNI=20.085632
CMO=0.28854226
CCU=0.24114047
CN=7.0332636E-2
CFE=52.272887
CM23=0.47294685
POLY_3:
POLY_3: enter-symb
Constant, variable, function or table? /FUNCTION/: FUNCTION
Name: tc=t-273.15;
POLY_3:
POLY_3: @@ Enter empirical parameters as function of temperature
POLY_3: ent func bc=575-0.3686*tc;
POLY_3: ent func bsi=24.76+1.129e-4*tc*tc-0.09*tc;
POLY_3: ent func bmn=-1.4-0.007*tc;
POLY_3: ent func bcr=0.3-tc*7e-4;
POLY_3: ent func bni=5.3-tc*3.3e-3;
POLY_3: ent func bmo=6-tc*3.3e-3;
POLY_3: ent func bcu=-14+0.0116*tc;
POLY_3: ent func bn=937-2.74e-6*tc*tc*tc+5.24e-3*tc*tc-3.08*tc;
POLY_3: ent func bm23=48+0.0135*tc;
POLY_3: ent func at=1.68+4.248e-6*tc*tc-4.33e-3*tc;
POLY_3:
POLY_3: li-symb *
DEFINED FUNCTIONS AND VARIABLES%
CC%=100*W(FCC_A1,C)
CSI%=100*W(FCC_A1,SI)
CMN%=100*W(FCC_A1,MN)
CCR%=100*W(FCC_A1,CR)
CNI%=100*W(FCC_A1,NI)
CMO%=100*W(FCC_A1,MO)
CCU%=100*W(FCC_A1,CU)
CN%=100*W(FCC_A1,N)
CFE%=100*W(FCC_A1,FE)
CM23%=100*BPW(M23C6)
TC=T-273.15
BC=575-.3686*TC
BSI=24.76+1.129E-04*TC*TC-.09*TC
BMN=-1.4-.007*TC
BCR=.3-TC*7E-04
BNI=5.3-TC*.0033
BMO=6-TC*.0033
BCU=-14+.0116*TC
BN=937-2.74E-06*TC*TC*TC+.00524*TC*TC-3.08*TC
BM23=48+.0135*TC
AT=1.68+4.248E-06*TC*TC-.00433*TC
POLY_3:
POLY_3: eval
Name(s): *
CC=6.4116133E-2
CSI=1.3061775
CMN=1.3037802
CCR=24.367392
CNI=20.085632
CMO=0.28854226
CCU=0.24114047
CN=7.0332636E-2
CFE=52.272887
CM23=0.47294685
TC=1079.85
BC=176.96729

```

```

BSI=59.223483
BMN=-8.95895
BCR=-0.455895
BNI=1.736495
BMO=2.436495
BCU=-1.47374
BN=271.12745
BM23=62.577975
AT=1.9577404
POLY_3:
POLY_3: @@ Enter an empirical expression for the proof strength combining
POLY_3: @@ the variables and function parameters previously entered.
POLY_3: ent
Constant, variable, function or table? /FUNCTION/: FUNCTION
Name: rp1
Function: at+bc*cc+bsi*csi+bm*cmn+bni*cn;
POLY_3:
POLY_3: ent
Constant, variable, function or table? /FUNCTION/: FUNCTION
Name: rp2
Function: bcr*ccr+bmo*cmo+bcu*ccu+bn*cn+bm23*cm23;
POLY_3:
POLY_3: ent func rp02=rp1+rp2;
POLY_3:
POLY_3: eval
Name(s): *
CC=6.4116133E-2
CSI=1.3061775
CMN=1.3037802
CCR=24.367392
CNI=20.085632
CMO=0.28854226
CCU=0.24114047
CN=7.0332636E-2
CFE=52.272887
CM23=0.47294685
TC=1079.85
BC=176.96729
BSI=59.223483
BMN=-8.95895
BCR=-0.455895
BNI=1.736495
BMO=2.436495
BCU=-1.47374
BN=271.12745
BM23=62.577975
AT=1.9577404
RP1=113.85868
RP2=37.903846
RP02=151.76252
POLY_3:
POLY_3: @@ turn off the global minimization calculation and suspend
POLY_3: @@ all phases except fcc_al#1. This will speed up the calculation
POLY_3: @@ and doesn't affect the results.
POLY_3: advanced
Which option? /STEP AND MAP/: glo
Settings for global minimization:
Use global minimization as much as possible /Y/: n,,,
POLY_3:
POLY_3: c-s phase
Phase name(s): *
Status: /ENTERED/: sus
POLY_3:
POLY_3: c-s phase fcc_al#1=enter 1
POLY_3:
POLY_3: s-c t=500
POLY_3: c-e
Global equilibrium calculation turned off, you can turn it on with
ADVANCED OPTIONS GLOBAL MINIMIZATION Y,,,,,,
7 ITS, CPU TIME USED 0 SECONDS
POLY_3: l-e,,,
Output from POLY-3, equilibrium = 1, label A0 , database: TCFE7

Conditions:
P=1E5, N=1, T=500, W(C)=9E-4, W(N)=7E-4, W(CR)=0.246, W(NI)=0.2,
W(MN)=1.3E-2, W(SI)=1.3E-2, W(CU)=2.4E-3, W(MO)=3E-3
DEGREES OF FREEDOM 0

Temperature 500.00 K ( 226.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 5.44622E+01
Total Gibbs energy -1.87430E+04, Enthalpy 9.33796E+03, Volume 7.00887E-06

Component      Moles      W-Fraction  Activity   Potential  Ref.stat
C               4.0809E-03  9.0000E-04  6.3735E-02 -1.1445E+04 SER
CR              2.5767E-01  2.4600E-01  2.3975E-01 -5.9371E+03 SER
CU              2.0569E-03  2.4000E-03  6.2527E-01 -1.9521E+03 SER
FE              5.0808E-01  5.2100E-01  3.3960E-02 -1.4062E+04 SER
MN              1.2887E-02  1.3000E-02  6.1504E-06 -4.9883E+04 SER
MO              1.7030E-03  3.0000E-03  6.4768E-02 -1.1378E+04 SER
N               2.7217E-03  7.0000E-04  5.4203E-14 -1.2699E+05 SER
NI              1.8559E-01  2.0000E-01  9.0077E-04 -2.9152E+04 SER
SI              2.5209E-02  1.3000E-02  1.2109E-15 -1.4279E+05 SER

FCC A1          Status ENTERED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 5.4462E+01, Volume fraction 1.0000E+00 Mass fractions:
FE 5.21000E-01 SI 1.30000E-02 CU 2.40000E-03
CR 2.46000E-01 MN 1.30000E-02 C 9.00000E-04
NI 2.00000E-01 MO 3.00000E-03 N 7.00000E-04
POLY_3: l-st
Option /CPS/:
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS      REF. STATE      T(K)          P(Pa)
VA              ENTERED     SER
C               ENTERED     SER
CR              ENTERED     SER
CU              ENTERED     SER
FE              ENTERED     SER
MN              ENTERED     SER
MO              ENTERED     SER
N               ENTERED     SER
NI              ENTERED     SER
SI              ENTERED     SER
*** STATUS FOR ALL PHASES
PHASE          STATUS      DRIVING FORCE      MOLES

```

```

FCC_A1          ENTERED      0.000000E+00    1.000000E+00
SUSPENDED PHASES:
Z PHASE SIGMA SIC SI3N4 R PHASE P PHASE PI NI3TI NBNI3 MU PHASE MSI MN6N5
MN6N4 MC_SHP MC_ETA M7C3 M6C M5SI3 M5C2 M3SI M3C2 M23C6 LAVES_PHASE_C14
KSI CARBIDE KAPPA HCP_A3#2 HCP_A3 G_PHASE GRAPHITE FECN_CHI FE8SI2C FE4N_LP1
FE2SI FCC_A1#2 DIAMOND FCC_A4 CR3SI_CHI_A12 CEMENTITE BCC_A2 AL4C3 LIQUID GAS
*** STATUS FOR ALL SPECIES
C          ENTERED      C3          ENTERED      C6N1          ENTERED      N          ENTERED
C1N1      ENTERED      C3N1      ENTERED      C6N2          ENTERED      N2          ENTERED
C1N2_CNN  ENTERED      C4          ENTERED      C9N1          ENTERED      N3          ENTERED
C1N2_NCN  ENTERED      C4N1      ENTERED      CR          ENTERED      NI          ENTERED
C2         ENTERED      C4N2      ENTERED      CU          ENTERED      SI          ENTERED
C2N1_CCN  ENTERED      C5          ENTERED      FE          ENTERED      SI3N4      ENTERED
C2N1_CNC  ENTERED      C5N1      ENTERED      MN          ENTERED      SIN4/3     ENTERED
C2N2      ENTERED      C60          ENTERED      MO          ENTERED      VA          ENTERED
POLY_3:Hit RETURN to continue
POLY_3: s-a-v l t
Min value /0/: 200
Max value /1/: 1000
Increment /20/: 10
POLY_3:
POLY_3: save tcex44 y
POLY_3: @@ Step in temperature in order to evaluate proof strength
POLY_3: @@ as function of temperature.
POLY_3: step normal
No initial equilibrium, using default
Step will start from axis value 500.000
POLY has calculated initial equilibrium

Phase Region from 500.000 for:
FCC_A1
Terminating at 1000.000
Calculated 53 equilibria

Phase Region from 500.000 for:
FCC_A1
Terminating at 200.000
Calculated 33 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex44\tcex
44.POLY3
POLY_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

```

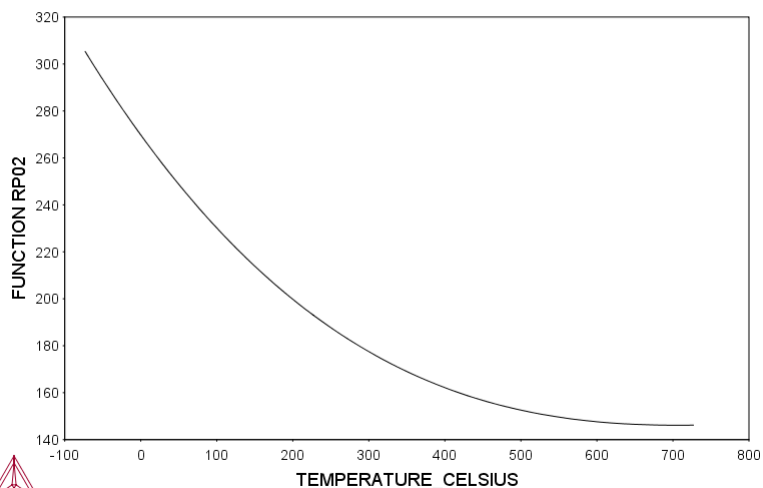
```

POST: s-d-a y rp02
POST: s-d-a x t-c
POST:
POST: set-title example 44a
POST: plot

```

example 44a

2016.05.16.14.37.58  
TCFE7: C, CR, CU, FE, MN, MO, N, NI, SI  
P=1E5, N=1, W(C)=9E-4, W(N)=7E-4, W(CR)=0.246, W(NI)=0.2, W(MN)=1.3E-2, W(SI)=1.3E-2, W(CU)=2.4E-3, W(MO)=3E-3



```

POST:
POST:Hit RETURN to continue
POST:
POST: s-s-s x n 0 500
POST:
POST: set-ras y
POST:
POST: set-title example 44b
POST:
POST: plot

```

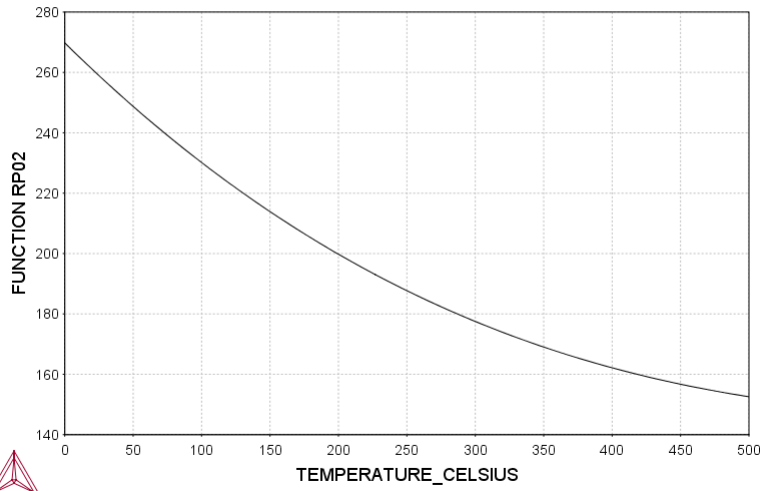


### example 44b

2016.05.16.14.38.00

TCFE7: C, CR, CU, FE, MN, MO, N, NI, SI

P=1E5, N=1., W(C)=9E-4, W(N)=7E-4, W(CR)=0.246, W(NI)=0.2, W(MN)=1.3E-2, W(SI)=1.3E-2, W(CU)=2.4E-3, W(MO)=3E-3



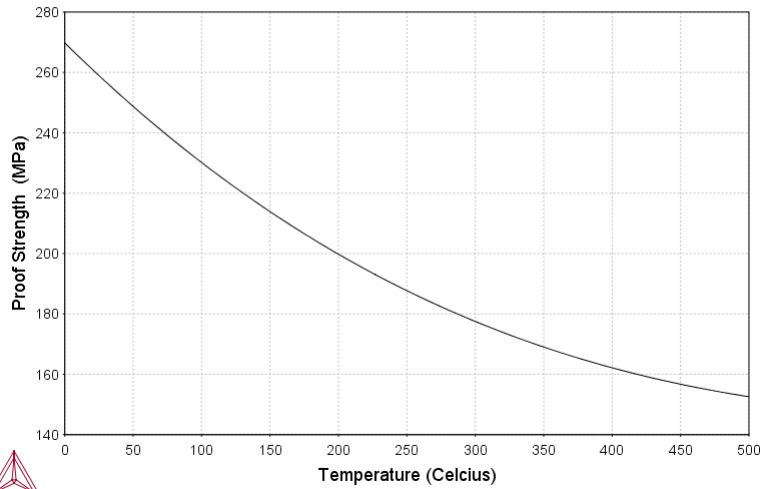
```
POST:
POST:Hit RETURN to continue
POST:
POST: set-axis-text-status
AXIS (X, Y OR Z) : y
AUTOMATIC AXIS TEXT (Y OR N) /N/: n
AXIS TEXT : Proof Strength (MPa)
POST:
POST: set-axis-text-status
AXIS (X, Y OR Z) : x
AUTOMATIC AXIS TEXT (Y OR N) /N/: n
AXIS TEXT : Temperature (Celcius)
POST:
POST: set-title example 44c
POST:
POST: plot
```

### example 44c

2016.05.16.14.38.02

TCFE7: C, CR, CU, FE, MN, MO, N, NI, SI

P=1E5, N=1., W(C)=9E-4, W(N)=7E-4, W(CR)=0.246, W(NI)=0.2, W(MN)=1.3E-2, W(SI)=1.3E-2, W(CU)=2.4E-3, W(MO)=3E-3



```
POST:
POST: set-inter
POST:
```

## tcex45

### About Stockholm, Sweden

Software (build 9533) running on WinNT 64-bit wordlength  
Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118  
License library version: 8.5.1.0017  
Linked: Mon May 16 09:31:44 2016

```
SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex45\tcex45.TCM" set-echo
```

```
SYS: @@  
SYS: @@ 3D-Diagram  
SYS: @@ with the gamma volume in the Fe-Cr-C system  
SYS: @@  
SYS: @@ This file calculates the gamma volume in the fe-cr-c system.  
SYS: @@ Please note that in order to view the generated file, tcex45.wrl,  
SYS: @@ it's necessary to install a WRML(Virtual Reality Modelling  
SYS: @@ Language) viewer to the web browser in use. WRML viewers can be  
SYS: @@ downloaded from e.g. www.parallelgraphics.com and www.sim.no  
SYS:  
SYS: set-log ex45,,,  
SYS:  
SYS: @@ Start with calculating the Fe-C side of the diagram  
SYS: go data  
... the command in full is GOTO_MODULE  
THERMODYNAMIC DATABASE module  
Current database: Steels/Fe-Alloys v8.0
```

```
VA DEFINED  
L12_FCC B2_BCC B2_VACANCY  
HIGH_SIGMA DICTRA_FCC_A1 REJECTED
```

```
TDB_TCFE8: sw FEDEMO  
... the command in full is SWITCH_DATABASE  
Current database: Iron Demo Database
```

```
VA /- DEFINED  
TDB_FEDEMO: def-sys fe c  
... the command in full is DEFINE_SYSTEM  
FE C DEFINED  
TDB_FEDEMO: get  
... the command in full is GET_DATA  
REINITIATING GES5 .....  
ELEMENTS .....  
SPECIES .....  
PHASES .....  
... the command in full is AMEND_PHASE_DESCRIPTION  
... the command in full is AMEND_PHASE_DESCRIPTION  
... the command in full is AMEND_PHASE_DESCRIPTION  
PARAMETERS ...  
FUNCTIONS ...
```

List of references for assessed data

'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'  
'B. Uhrenius (1993-1994), International journal of refractory metals and hard mater, Vol. 12, pp. 121-127; Molar volumes'  
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89; Molar volumes'  
'X.-G. Lu et al. Calphad 29 (2005) 49-55, Fe P-T diagram'  
'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C -FE'  
'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'  
'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo -C, C-Mn'  
'J.-O. Andersson, Calphad, 12 (1988), 9-23; TRITA 0321 (1986); C -FE-MO'  
'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equil., 19 (1998), 441-448; Fe-Ti'  
'J.-O. Andersson, Metall. Trans. A, 19A (1988), 627-636 TRITA 0207 (1986); C-CR-FE'  
'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'  
'P. Villars and L.D. Calvert (1985). Pearsons handbook of crystallographic data for intermetallic phases. Metals park, Ohio. American Society for Metals; Molar volumes'  
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'

-OK-

```
TDB_FEDEMO:
```

```
TDB_FEDEMO: go poly  
... the command in full is GOTO_MODULE
```

```
POLY version 3.32  
POLY_3: s-c t=1373  
... the command in full is SET_CONDITION  
POLY_3: se-co n=1,p=1e5  
... the command in full is SET_CONDITION  
POLY_3: se-co x(c)=2e-2  
... the command in full is SET_CONDITION  
POLY_3: c-e  
... the command in full is COMPUTE_EQUILIBRIUM  
Using global minimization procedure  
Calculated 1963 grid points in 0 s  
Found the set of lowest grid points in 0 s  
Calculated POLY solution 0 s, total time 0 s
```

```
POLY_3:  
POLY_3: s-a-v 1 x(c) 0 1 .01  
... the command in full is SET_AXIS_VARIABLE  
POLY_3: s-a-v 2 t 800 1800 10  
... the command in full is SET_AXIS_VARIABLE
```

```
POLY_3:  
POLY_3: advanced  
... the command in full is ADVANCED_OPTIONS
```

Which option? /STEP\_AND\_MAP/: present

Phase name /NONE/: fcc\_a1

```
POLY_3:  
POLY_3: save tcex45 y  
... the command in full is SAVE_WORKSPACES  
POLY_3: map
```

Version 3 mapping is selected  
Generating start equilibrium 1  
Generating start equilibrium 2  
Generating start equilibrium 3  
Generating start equilibrium 4  
Generating start equilibrium 5  
Generating start equilibrium 6

Generating start equilibrium 7  
Generating start equilibrium 8  
Generating start equilibrium 9  
Generating start equilibrium 10  
Generating start equilibrium 11  
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1  
Generating start point 2  
Generating start point 3  
Generating start point 4  
Generating start point 5  
Generating start point 6  
Generating start point 7  
Generating start point 8  
Generating start point 9  
Generating start point 10

Working hard

Generating start point 11  
Generating start point 12  
Generating start point 13  
Generating start point 14  
Generating start point 15  
Generating start point 16  
Generating start point 17  
Generating start point 18  
Generating start point 19  
Generating start point 20

Working hard

Generating start point 21  
Generating start point 22  
Generating start point 23  
Generating start point 24  
Generating start point 25  
Generating start point 26  
Generating start point 27  
Generating start point 28  
Generating start point 29  
Generating start point 30

Working hard

Generating start point 31  
Generating start point 32

Phase region boundary 1 at: 5.236E-01 1.137E+03  
FCC\_A1  
\*\* GRAPHITE  
Calculated. 14 equilibria

Phase region boundary 2 at: 5.155E-01 1.011E+03  
\*\* BCC\_A2  
FCC\_A1  
\*\* GRAPHITE

Phase region boundary 3 at: 1.587E-02 1.011E+03  
\*\* BCC\_A2  
FCC\_A1  
Calculated. 38 equilibria

Phase region boundary 4 at: 5.155E-01 1.011E+03  
FCC\_A1  
\*\* GRAPHITE  
Calculated. 43 equilibria

Phase region boundary 5 at: 5.439E-01 1.427E+03  
\*\* LIQUID  
FCC\_A1  
\*\* GRAPHITE

Phase region boundary 6 at: 1.310E-01 1.427E+03  
\*\* LIQUID  
FCC\_A1  
Calculated. 36 equilibria

Phase region boundary 7 at: 1.599E-02 1.768E+03  
\*\* LIQUID  
\*\* BCC\_A2  
FCC\_A1

Phase region boundary 8 at: 6.113E-03 1.768E+03  
\*\* BCC\_A2  
FCC\_A1  
Calculated. 26 equilibria

Phase region boundary 9 at: 5.236E-01 1.137E+03  
FCC\_A1  
\*\* GRAPHITE  
Calculated. 30 equilibria  
Terminating at known equilibrium

Phase region boundary 10 at: 5.236E-01 1.137E+03  
FCC\_A1  
\*\* GRAPHITE  
Calculated. 14 equilibria  
Terminating at known equilibrium

Phase region boundary 11 at: 5.236E-01 1.137E+03  
FCC\_A1  
\*\* GRAPHITE  
Calculated. 30 equilibria  
Terminating at known equilibrium

Phase region boundary 12 at: 1.216E-01 1.463E+03  
\*\* LIQUID  
FCC\_A1  
Calculated. 5 equilibria  
Terminating at known equilibrium

Phase region boundary 13 at: 1.216E-01 1.463E+03  
\*\* LIQUID  
FCC\_A1  
Calculated. 32 equilibria  
Terminating at known equilibrium

```

*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex45\tcex
45.POLY3
CPU time for mapping                      1 seconds
POLY_3:
POLY_3: post

```

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

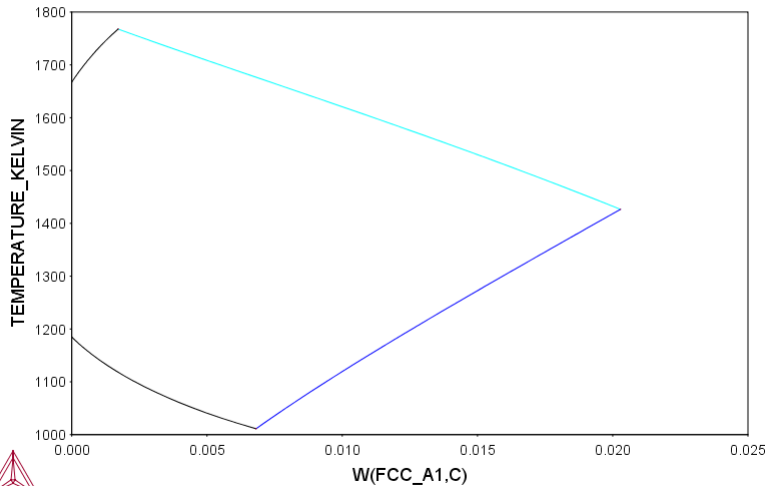
```

POST: s-d-a x w(fcc_al,c)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y te-k
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 45a
POST: plot
... the command in full is PLOT DIAGRAM

```

example 45a

2016.05.16.14.39.33  
FEDEMO: C, FE  
N=1, P=1E5



```

POST:
POST:Hit RETURN to continue
POST:
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the C content in the fcc_al phase, in the second Cr content which is "zero"
POST: @@ here, and in the last column the temperature.
POST: e-sym tab tabl
... the command in full is ENTER_SYMBOL
Variable(s): W(fcc_al,c),zero,T
&
POST: @@ Save the tabulated data on file
POST: tab tabl fec.tab
... the command in full is TABULATE
POST: back
POLY_3:
POLY_3: @@ Next step is to calculate the Fe-Cr side of the diagram
POLY_3: go data
... the command in full is GOTO_MODULE
TDB_FEDEMO: rej-sys
... the command in full is REJECT
VA          /- DEFINED
REINITIATING GES5 .....
TDB_FEDEMO: de-sys fe cr
... the command in full is DEFINE_SYSTEM
FE          CR DEFINED
TDB_FEDEMO: get
... the command in full is GET_DATA
REINITIATING GES5 .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

```

List of references for assessed data

'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'  
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'  
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;  
Molar volumes'  
'X.-G. Lu et al. Calphad 29 (2005) 49-55, Fe P-T diagram'  
'B.-J. Lee, Calphad (1993); revision of Fe-Cr and Fe-Ni liquid'  
'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'  
'J.-O. Andersson and B. Sundman, Calphad, 11 (1987), 83-92; TRITA 0270  
(1986); CR-FE'  
'P. Gustafson, TRITA-MAC 342 (1987); CR-FE-W'  
'J.-O. Andersson, Metall. Trans. A, 19A (1988), 1385-1394; TRITA 0322  
(1986); CR-FE-MO'  
'K. Frisk, Metall. Trans. A, 21A (1990), 2477-2488; TRITA 0409 (1989); CR  
-FE-N'  
'N. Saunders, COST 507 Report (1998); Cr-Ti'  
'B.-J. Lee, estimated parameter 1999'  
'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equil., 19 (1998),  
441-448; Fe-Ti'  
'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New  
Sigma model'

```

-OK-
TDB_FEDEMO:
TDB_FEDEMO: go poly

```

```

... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3: s-c t=1373
... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
... the command in full is SET_CONDITION
POLY_3: se-co x(cr)=2e-2
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 6005 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY_3:
POLY_3: s-a-v 1 x(cr) 0 1 .01
... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 t 800 1800 10
... the command in full is SET_AXIS_VARIABLE
POLY_3:
POLY_3: advanced
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /NONE/: fcc_a1
POLY_3:
POLY_3: save tcex45 y
... the command in full is SAVE_WORKSPACES

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

```

```

POLY_3: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

```

Organizing start points

Using ADDED start equilibria

```

Working hard
Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard
Generating start point 21
Generating start point 22
Generating start point 23
Generating start point 24
Generating start point 25
Generating start point 26
Generating start point 27
Generating start point 28

```

```

Phase region boundary 1 at: 1.067E-02 1.169E+03
BCC_A2
** FCC_A1
Calculated 11 equilibria

Phase region boundary 2 at: 1.067E-02 1.169E+03
BCC_A2
** FCC_A1
Calculated 92 equilibria

Phase region boundary 3 at: 4.325E-02 1.137E+03
BCC_A2
** FCC_A1
Calculated 83 equilibria

Phase region boundary 4 at: 4.325E-02 1.137E+03
BCC_A2
** FCC_A1
Calculated 16 equilibria

Phase region boundary 5 at: 1.006E-01 1.137E+03
BCC_A2
** FCC_A1
Calculated 32 equilibria

Phase region boundary 6 at: 1.006E-01 1.137E+03
BCC_A2
** FCC_A1
Calculated 75 equilibria

Phase region boundary 7 at: 1.051E-01 1.463E+03

```

```

** BCC_A2
FCC_A1
Calculated                63 equilibria

Phase region boundary  8 at:  1.051E-01  1.463E+03
** BCC_A2
FCC_A1
Calculated                38 equilibria

Phase region boundary  9 at:  1.051E-01  1.463E+03
** BCC_A2
FCC_A1
Calculated                63 equilibria

Phase region boundary 10 at:  1.051E-01  1.463E+03
** BCC_A2
FCC_A1
Calculated                38 equilibria

Phase region boundary 11 at:  9.912E-03  1.665E+03
** BCC_A2
FCC_A1
Calculated                15 equilibria

Phase region boundary 12 at:  9.912E-03  1.665E+03
** BCC_A2
FCC_A1
Calculated                88 equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex45\tcex
45.POLY3
CPU time for mapping                2 seconds

```

POLY\_3:  
POLY\_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

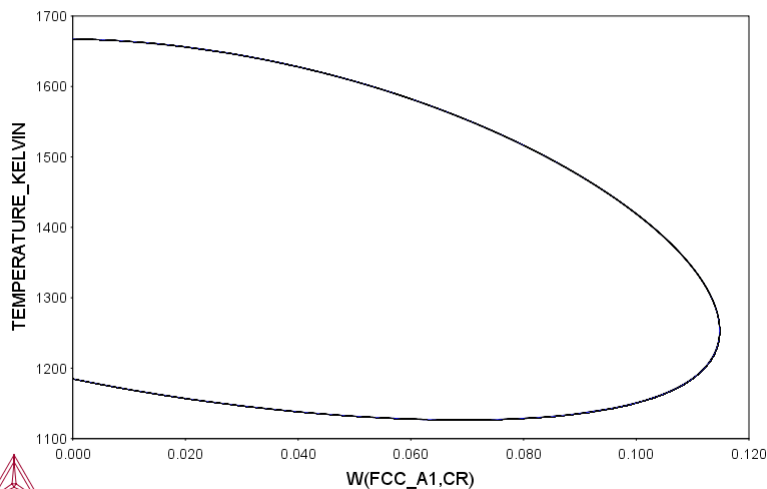
Setting automatic diagram axes

```

POST: s-d-a x W(fcc_a1,cr)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y te-k
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 45b
POST:
POST: plot
... the command in full is PLOT DIAGRAM
                                example 45b

```

2016.05.16.14.39.37  
FEDEMO: CR, FE  
N=1, P=1E5



```

POST:
POST:
POST: Hit RETURN to continue
POST:
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the C content in the fcc_a1 phase, in the second the Cr content,
POST: @@ and in the last column the temperature.
POST: e-sym tab tabl
... the command in full is ENTER_SYMBOL
Variable(s): zero,W(fcc_a1,cr),T
&
POST: @@ Save the tabulated data on file
POST: tab tabl fecr.tab
... the command in full is TABULATE
POST:
POST: @@ Now let's calculate the ternary projection of the fcc_a1 phase
POST: back
POLY_3: go data
... the command in full is GOTO_MODULE
TDB_FEDEMO: rej-sys
... the command in full is REJECT
VA /- DEFINED
REINITIATING GES5 .....
TDB_FEDEMO: de-sys fe cr c
... the command in full is DEFINE_SYSTEM
FE CR C
DEFINED
TDB_FEDEMO: get
... the command in full is GET_DATA
REINITIATING GES5 .....
ELEMENTS .....
SPECIES .....
PHASES .....

```

```

... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

```

List of references for assessed data

```

'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'
'B. Uhrenius (1993-1994), International journal of refractory metals and
  hard mater, Vol. 12, pp. 121-127; Molar volumes'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
  Molar volumes'
'X.-G. Lu et al. Calphad 29 (2005) 49-55, Fe P-T diagram'
'J.-O. Andersson, Calphad, 11 (1987), 271-276; TRITA 0314; C-CR'
'B.-J. Lee, Calphad (1993); revision of Fe-Cr and Fe-Ni liquid'
'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
  -FE'
'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo -C, C-Mn'
'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'
'J.-O. Andersson, Metall. Trans. A, 19A (1988), 627-636 TRITA 0207 (1986);
  C-CR-Fe'
'J.-O. Andersson and B. Sundman, Calphad, 11 (1987), 83-92; TRITA 0270
  (1986); CR-Fe'
'P. Villars and L.D. Calvert (1985). Pearsons handbook of crystallographic
  data for intermetallic phases. Metals park, Ohio. American Society for
  Metals; Molar volumes'
'J. Bratberg, Z. Metallkd., Vol 96 (2005), 335-344; Fe-Cr-Mo-C'
'P. Gustafson, TRITA-MAC 342 (1987); CR-Fe-W'
'J.-O. Andersson, Metall. Trans. A, 19A (1988), 1385-1394; TRITA 0322
  (1986); CR-Fe-MO'
'C. Qiu, ISIJ International, 32 (1992), 1117-1127; C-Cr-Fe-Mo'
'P. Gustafson, Metall. Trans. A, 19A (1988), 2547-2554; TRITA-MAC 348,
  (1987); C-CR-Fe-W'
'K. Frisk, Metall. Trans. A, 21A (1990), 2477-2488; TRITA 0409 (1989); CR
  -FE-N'
'J.-O. Andersson, Calphad, 12 (1988), 9-23; TRITA 0321 (1986); C -FE-MO'
'N. Saunders, COST 507 Report (1998); Cr-Ti'
'B.-J. Lee, estimated parameter 1999'
'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equil., 19 (1998),
  441-448; Fe-Ti'
'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
  Sigma model'

```

-OK-

**TDB\_FEDEMO:**

**TDB\_FEDEMO:** go poly

```

... the command in full is GOTO_MODULE

```

POLY version 3.32

**POLY\_3:** s-c t=1373

```

... the command in full is SET_CONDITION

```

**POLY\_3:** se-co n=1,p=1e5

```

... the command in full is SET_CONDITION

```

**POLY\_3:** se-co x(c)=.01

```

... the command in full is SET_CONDITION

```

**POLY\_3:** se-co x(cr)=2e-2

```

... the command in full is SET_CONDITION

```

**POLY\_3:** c-e

```

... the command in full is COMPUTE_EQUILIBRIUM

```

Using global minimization procedure

```

Calculated      16532 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution      0 s, total time    0 s

```

**POLY\_3:**

**POLY\_3:** s-a-v 1 x(c) 0 1 .01

```

... the command in full is SET_AXIS_VARIABLE

```

**POLY\_3:** s-a-v 2 x(cr) 0 1 .01

```

... the command in full is SET_AXIS_VARIABLE

```

**POLY\_3:**

**POLY\_3:** se-con t=1050

```

... the command in full is SET_CONDITION

```

**POLY\_3:** c-e

```

... the command in full is COMPUTE_EQUILIBRIUM

```

Using global minimization procedure

```

Calculated      16532 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution      0 s, total time    0 s

```

**POLY\_3:** add-in 1

```

... the command in full is ADD_INITIAL_EQUILIBRIUM

```

**POLY\_3:**

**POLY\_3:** se-con t=1100

```

... the command in full is SET_CONDITION

```

**POLY\_3:** c-e

```

... the command in full is COMPUTE_EQUILIBRIUM

```

Using global minimization procedure

```

Calculated      16532 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution      0 s, total time    0 s

```

**POLY\_3:** add-in 1

```

... the command in full is ADD_INITIAL_EQUILIBRIUM

```

**POLY\_3:**

**POLY\_3:** se-con t=1200

```

... the command in full is SET_CONDITION

```

**POLY\_3:** c-e

```

... the command in full is COMPUTE_EQUILIBRIUM

```

Using global minimization procedure

```

Calculated      16532 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution      0 s, total time    0 s

```

**POLY\_3:** add-in 1

```

... the command in full is ADD_INITIAL_EQUILIBRIUM

```

**POLY\_3:**

**POLY\_3:** se-con t=1300

```

... the command in full is SET_CONDITION

```

**POLY\_3:** c-e

```

... the command in full is COMPUTE_EQUILIBRIUM

```

Using global minimization procedure

```

Calculated      16532 grid points in          1 s
Found the set of lowest grid points in          0 s
Calculated POLY solution      0 s, total time    1 s

```

**POLY\_3:** add-in 1

```

... the command in full is ADD_INITIAL_EQUILIBRIUM

```

```

POLY_3:
POLY_3: se-con t=1400
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      16532 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution      0 s, total time    0 s
POLY_3: add-in 1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=1500
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      16532 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution      0 s, total time    0 s
POLY_3: add-in 1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=1600
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      16532 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution      0 s, total time    0 s
POLY_3: add-in 1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=1700
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      16532 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution      0 s, total time    0 s
POLY_3: add-in 1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: advanced
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /NONE/: fcc_a1
POLY_3:
POLY_3: save fecrc y
... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3: map
Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point  1
Generating start point  2
Generating start point  3
Generating start point  4
Generating start point  5
Generating start point  6
Generating start point  7
Generating start point  8
Generating start point  9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17

Phase region boundary  1 at:  1.591E-01  2.037E-01
  FCC_A1
  ** M7C3
Calculated.              5 equilibria

Phase region boundary  2 at:  1.629E-01  1.729E-01
  ** CEMENTITE
  FCC_A1
  ** M7C3

Phase region boundary  3 at:  1.379E-01  8.893E-02
  ** CEMENTITE
  FCC_A1
Calculated.              8 equilibria

Phase region boundary  4 at:  1.434E-01  1.958E-02
  ** CEMENTITE
  FCC_A1
  ** GRAPHITE

Phase region boundary  5 at:  5.184E-01  1.508E-03
  FCC_A1
  ** GRAPHITE
Calculated              9 equilibria

Phase region boundary  6 at:  1.629E-01  1.729E-01
  FCC_A1
  ** M7C3
Calculated.              5 equilibria

Phase region boundary  7 at:  1.591E-01  2.037E-01
  ** BCC_A2
  FCC_A1
  ** M7C3

Phase region boundary  8 at:  9.381E-03  1.618E-02

```



```

** BCC_A2
FCC_A1
Calculated
12 equilibria

Phase region boundary 9 at: 9.381E-03 1.618E-02
** BCC_A2
** FCC_A1
Calculated
14 equilibria

Phase region boundary 10 at: 1.633E-01 1.837E-01
FCC_A1
** M7C3
Calculated.
3 equilibria

Phase region boundary 11 at: 1.652E-01 1.705E-01
** CEMENTITE
FCC_A1
** M7C3

Phase region boundary 12 at: 1.402E-01 9.104E-02
** CEMENTITE
FCC_A1
Calculated.
9 equilibria

Phase region boundary 13 at: 1.466E-01 1.470E-02
** CEMENTITE
FCC_A1
** GRAPHITE

Phase region boundary 14 at: 5.216E-01 1.359E-03
FCC_A1
** GRAPHITE
Calculated
11 equilibria

Phase region boundary 15 at: 1.652E-01 1.705E-01
FCC_A1
** M7C3
Calculated.
19 equilibria

Phase region boundary 16 at: 1.521E-01 3.433E-01
FCC_A1
** M23C6
** M7C3

Phase region boundary 17 at: 1.055E-01 3.150E-01
FCC_A1
** M23C6
Calculated.
2 equilibria

Phase region boundary 18 at: 1.054E-01 3.213E-01
** BCC_A2
FCC_A1
** M23C6

Phase region boundary 19 at: 2.070E-03 1.073E-01
** BCC_A2
FCC_A1
Calculated
23 equilibria

Phase region boundary 20 at: 1.633E-01 1.837E-01
FCC_A1
** M7C3
Calculated.
17 equilibria
Terminating at known equilibrium

Phase region boundary 21 at: 1.472E-01 7.619E-02
** CEMENTITE
FCC_A1
Calculated.
8 equilibria

Phase region boundary 22 at: 1.534E-01 7.611E-03
** CEMENTITE
FCC_A1
** GRAPHITE

Phase region boundary 23 at: 5.284E-01 9.641E-04
FCC_A1
** GRAPHITE
Calculated
11 equilibria

Phase region boundary 24 at: 1.534E-01 7.611E-03
** CEMENTITE
FCC_A1
Calculated.
10 equilibria

Phase region boundary 25 at: 1.456E-01 9.385E-02
** CEMENTITE
FCC_A1
** M7C3

Phase region boundary 26 at: 1.706E-01 1.651E-01
FCC_A1
** M7C3
Calculated.
20 equilibria

Phase region boundary 27 at: 1.540E-01 3.475E-01
FCC_A1
** M23C6
** M7C3

Phase region boundary 28 at: 1.074E-01 3.204E-01
FCC_A1
** M23C6
Calculated.
5 equilibria

Phase region boundary 29 at: 1.065E-01 3.518E-01
** BCC_A2
FCC_A1
** M23C6

Phase region boundary 30 at: 3.537E-03 1.631E-01
** BCC_A2
FCC_A1
Calculated
17 equilibria

Phase region boundary 31 at: 1.472E-01 7.619E-02

```

```

** CEMENTITE
FCC_A1
Calculated.          3 equilibria
Terminating at known equilibrium

Phase region boundary 32 at: 1.555E-01 5.938E-02
** CEMENTITE
FCC_A1
Calculated.          8 equilibria

Phase region boundary 33 at: 1.603E-01 4.094E-03
** CEMENTITE
FCC_A1
** GRAPHITE

Phase region boundary 34 at: 5.353E-01 6.720E-04
FCC_A1
** GRAPHITE
Calculated          11 equilibria

Phase region boundary 35 at: 1.603E-01 4.094E-03
** CEMENTITE
FCC_A1
Calculated.          11 equilibria

Phase region boundary 36 at: 1.523E-01 9.416E-02
** CEMENTITE
FCC_A1
** M7C3

Phase region boundary 37 at: 1.773E-01 1.579E-01
FCC_A1
** M7C3
Calculated.          21 equilibria

Phase region boundary 38 at: 1.566E-01 3.575E-01
FCC_A1
** M23C6
** M7C3

Phase region boundary 39 at: 1.100E-01 3.333E-01
FCC_A1
** M23C6
Calculated.          3 equilibria

Phase region boundary 40 at: 1.093E-01 3.506E-01
** BCC_A2
FCC_A1
** M23C6

Phase region boundary 41 at: 6.971E-03 1.843E-01
** BCC_A2
FCC_A1
Calculated          15 equilibria

Phase region boundary 42 at: 1.555E-01 5.938E-02
** CEMENTITE
FCC_A1
Calculated.          5 equilibria
Terminating at known equilibrium

Phase region boundary 43 at: 1.641E-01 4.814E-02
** CEMENTITE
FCC_A1
Calculated.          6 equilibria

Phase region boundary 44 at: 1.675E-01 4.450E-03
** CEMENTITE
FCC_A1
** GRAPHITE

Phase region boundary 45 at: 5.425E-01 9.066E-04
FCC_A1
** GRAPHITE
Calculated          12 equilibria

Phase region boundary 46 at: 1.675E-01 4.450E-03
** CEMENTITE
FCC_A1
Calculated.          10 equilibria

Phase region boundary 47 at: 1.603E-01 9.101E-02
** CEMENTITE
FCC_A1
** M7C3

Phase region boundary 48 at: 1.853E-01 1.474E-01
FCC_A1
** M7C3
Calculated.          24 equilibria

Phase region boundary 49 at: 1.599E-01 3.696E-01
** BCC_A2
FCC_A1
** M7C3

Phase region boundary 50 at: 1.213E-02 2.017E-01
** BCC_A2
FCC_A1
Calculated          26 equilibria

Phase region boundary 51 at: 1.641E-01 4.814E-02
** CEMENTITE
FCC_A1
Calculated.          6 equilibria
Terminating at known equilibrium

Phase region boundary 52 at: 1.142E-01 2.495E-02
** LIQUID
FCC_A1
Calculated          16 equilibria

Phase region boundary 53 at: 1.142E-01 2.495E-02
** LIQUID
FCC_A1
Calculated.          6 equilibria

```

```

Phase region boundary 54 at: 1.177E-01 7.477E-02
** LIQUID
FCC_A1
** M7C3

Phase region boundary 55 at: 1.877E-01 1.707E-01
FCC_A1
** M7C3
Calculated. 21 equilibria

Phase region boundary 56 at: 1.645E-01 3.686E-01
** BCC_A2
FCC_A1
** M7C3

Phase region boundary 57 at: 1.810E-02 2.160E-01
** BCC_A2
FCC_A1
Calculated 20 equilibria

Phase region boundary 58 at: 1.177E-01 7.477E-02
** LIQUID
FCC_A1
Calculated 21 equilibria

Phase region boundary 59 at: 8.271E-02 2.328E-02
** LIQUID
FCC_A1
Calculated 11 equilibria

Phase region boundary 60 at: 8.271E-02 2.328E-02
** LIQUID
FCC_A1
Calculated. 23 equilibria

Phase region boundary 61 at: 6.085E-02 2.377E-01
** LIQUID
** BCC_A2
FCC_A1

Phase region boundary 62 at: 2.036E-02 2.062E-01
** BCC_A2
FCC_A1
Calculated 30 equilibria

Phase region boundary 63 at: 6.085E-02 2.377E-01
** LIQUID
FCC_A1
Calculated 35 equilibria

Phase region boundary 64 at: 4.494E-02 2.178E-02
** LIQUID
FCC_A1
Calculated 16 equilibria

Phase region boundary 65 at: 4.494E-02 2.178E-02
** LIQUID
FCC_A1
Calculated. 13 equilibria

Phase region boundary 66 at: 3.129E-02 1.383E-01
** LIQUID
** BCC_A2
FCC_A1

Phase region boundary 67 at: 1.259E-02 1.273E-01
** BCC_A2
FCC_A1
Calculated 25 equilibria

Phase region boundary 68 at: 3.129E-02 1.383E-01
** LIQUID
FCC_A1
Calculated 28 equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex45\fecr
c.POLY3
CPU time for mapping 5 seconds

POLY_3:
POLY_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

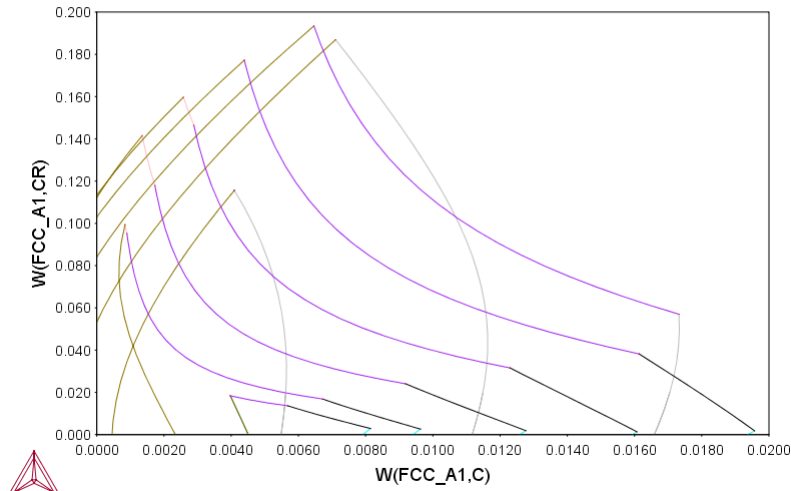
Setting automatic diagram axes

POST: s-d-a x W(fcc_a1,c)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y W(fcc_a1,cr)
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 45c
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

# example 45c

2016.05.16 14:39:50  
FEDEMO: C, CR, FE  
T=1700, N=1, P=1E5



```

POST:
POST:
POST:Hit RETURN to continue
POST: back
POLY_3:
POLY_3: s-a-v 1 x(c) 0 1 .01
... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(cr) 0 1 .01
... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 3 T 800 2000 5
... the command in full is SET_AXIS_VARIABLE
POLY_3: se-con x(cr)=.1
... the command in full is SET_CONDITION
POLY_3: se-con x(c)=.01
... the command in full is SET_CONDITION
POLY_3: se-con t=1373
... the command in full is SET_CONDITION
POLY_3:
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 16532 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY_3: ad-ini 1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: advanced
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /FCC_A1#1/: fcc_a1
POLY_3:
POLY_3: map
Version R mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18

Phase region boundary 1 at: 5.770E-04 1.292E-02 1.050E+03
BCC_A2
** FCC_A1
** M7C3
CALCULATED 7 EQUILIBRIA

Phase region boundary 2 at: 6.909E-04 7.705E-03 1.030E+03
BCC_A2
CEMENTITE
** FCC_A1
** M7C3

Phase region boundary 2 at: 3.000E-01 3.347E-01 1.030E+03
** CEMENTITE
** FCC_A1
M7C3
CALCULATED 89 EQUILIBRIA

Phase region boundary 2 at: 8.299E-02 4.133E-02 1.467E+03
LIQUID
** CEMENTITE
FCC_A1

```

```

** M7C3
SKIPPING LINE WITHOUT FCC_A1#1

Phase region boundary 2 at: 8.299E-02 4.133E-02 1.467E+03
** LIQUID
** CEMENTITE
FCC_A1
Terminating at diagram limit
CALCULATED 11 EQUILIBRIA

Phase region boundary 2 at: 8.299E-02 4.133E-02 1.467E+03
** LIQUID
FCC_A1
** M7C3
CALCULATED 31 EQUILIBRIA

Phase region boundary 2 at: 3.564E-02 2.106E-01 1.567E+03
** LIQUID
BCC_A2
FCC_A1
** M7C3
SKIPPING LINE WITHOUT FCC_A1#1

Phase region boundary 2 at: 3.564E-02 2.106E-01 1.567E+03
** LIQUID
** BCC_A2
FCC_A1
Terminating at diagram limit
CALCULATED 48 EQUILIBRIA

Phase region boundary 2 at: 3.564E-02 2.106E-01 1.567E+03
** BCC_A2
FCC_A1
** M7C3
CALCULATED 40 EQUILIBRIA

Phase region boundary 2 at: 1.817E-02 1.819E-01 1.380E+03
** BCC_A2
FCC_A1
M23C6
** M7C3
SKIPPING LINE WITHOUT FCC_A1#1

Phase region boundary 2 at: 1.817E-02 1.819E-01 1.380E+03
** BCC_A2
FCC_A1
** M23C6
CALCULATED 60 EQUILIBRIA

Phase region boundary 2 at: 3.999E-03 1.003E-01 1.096E+03
** BCC_A2
FCC_A1
** M23C6
M7C3
SKIPPING LINE WITHOUT FCC_A1#1

Phase region boundary 2 at: 3.999E-03 1.003E-01 1.096E+03
** BCC_A2
FCC_A1
** M7C3
Terminating at known equilibrium
CALCULATED 18 EQUILIBRIA

Phase region boundary 2 at: 3.999E-03 1.003E-01 1.096E+03
FCC_A1
** M23C6
** M7C3
Terminating at known equilibrium
CALCULATED 60 EQUILIBRIA

Phase region boundary 2 at: 6.909E-04 7.705E-03 1.030E+03
BCC_A2
** CEMENTITE
** FCC_A1
CALCULATED 7 EQUILIBRIA

Phase region boundary 2 at: 8.322E-04 1.593E-03 1.008E+03
BCC_A2
** CEMENTITE
** FCC_A1
GRAPHITE

Phase region boundary 2 at: 1.000E+00 0.000E+00 1.008E+03
** CEMENTITE
** FCC_A1
GRAPHITE
OUTSIDE AXIS LIMITS
Terminating at diagram limit
CALCULATED 6 EQUILIBRIA
SKIPPING LINE WITHOUT FCC_A1#1

Phase region boundary 2 at: 8.322E-04 1.593E-03 1.008E+03
BCC_A2
** FCC_A1
** GRAPHITE
Terminating at diagram limit
CALCULATED 8 EQUILIBRIA
SKIPPING LINE WITHOUT FCC_A1#1

Phase region boundary 2 at: 5.770E-04 1.292E-02 1.050E+03
BCC_A2
** FCC_A1
** M7C3
Terminating at known equilibrium
CALCULATED 15 EQUILIBRIA

Phase region boundary 2 at: 2.668E-02 2.000E-02 1.051E+03
** BCC_A2
FCC_A1
** M7C3
Terminating at known equilibrium
CALCULATED 7 EQUILIBRIA

Phase region boundary 2 at: 2.668E-02 2.000E-02 1.051E+03
** BCC_A2
FCC_A1

```

```

** M7C3
Terminating at known equilibrium
CALCULATED 14 EQUILIBRIA

Phase region boundary 2 at: 4.444E-02 2.000E-02 1.133E+03
** CEMENTITE
FCC_A1
** M7C3
Terminating at known equilibrium
CALCULATED 24 EQUILIBRIA

Phase region boundary 2 at: 4.444E-02 2.000E-02 1.133E+03
** CEMENTITE
FCC_A1
** M7C3
Terminating at known equilibrium
CALCULATED 70 EQUILIBRIA

Phase region boundary 2 at: 6.099E-02 2.000E-02 1.133E+03
** CEMENTITE
FCC_A1
** M7C3
Terminating at known equilibrium
CALCULATED 24 EQUILIBRIA

Phase region boundary 2 at: 6.099E-02 2.000E-02 1.133E+03
** CEMENTITE
FCC_A1
** M7C3
Terminating at known equilibrium
CALCULATED 70 EQUILIBRIA

Phase region boundary 2 at: 7.812E-02 2.000E-02 1.133E+03
** CEMENTITE
FCC_A1
** M7C3
Terminating at known equilibrium
CALCULATED 24 EQUILIBRIA

Phase region boundary 2 at: 7.812E-02 2.000E-02 1.133E+03
** CEMENTITE
FCC_A1
** M7C3
Terminating at known equilibrium
CALCULATED 70 EQUILIBRIA

Phase region boundary 2 at: 7.451E-02 2.000E-02 1.446E+03
** LIQUID
** CEMENTITE
FCC_A1
Terminating at diagram limit
CALCULATED 9 EQUILIBRIA

Phase region boundary 2 at: 7.451E-02 2.000E-02 1.446E+03
** LIQUID
** CEMENTITE
FCC_A1
Terminating at known equilibrium
CALCULATED 7 EQUILIBRIA

Phase region boundary 2 at: 5.118E-02 2.000E-02 1.446E+03
** LIQUID
** CEMENTITE
FCC_A1
Terminating at diagram limit
CALCULATED 9 EQUILIBRIA

Phase region boundary 2 at: 5.118E-02 2.000E-02 1.446E+03
** LIQUID
** CEMENTITE
FCC_A1
Terminating at known equilibrium
CALCULATED 7 EQUILIBRIA

Phase region boundary 2 at: 2.557E-02 2.000E-02 1.446E+03
** LIQUID
** CEMENTITE
FCC_A1
Terminating at diagram limit
CALCULATED 9 EQUILIBRIA

Phase region boundary 2 at: 2.557E-02 2.000E-02 1.446E+03
** LIQUID
** CEMENTITE
FCC_A1
Terminating at known equilibrium
CALCULATED 7 EQUILIBRIA

Phase region boundary 2 at: 2.829E-02 1.000E-01 1.096E+03
** BCC_A2
FCC_A1
** M7C3
Terminating at known equilibrium
CALCULATED 14 EQUILIBRIA

Phase region boundary 2 at: 2.829E-02 1.000E-01 1.096E+03
** BCC_A2
FCC_A1
** M7C3
Terminating at known equilibrium
*** LAST BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex45\fecr
c.POLY3
CPU time for mapping 2 seconds
POLY_3:
POLY_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes
POST: s-d-a x W(fcc_a1,c)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y W(fcc_a1,cr)
... the command in full is SET_DIAGRAM_AXIS

```

POST: set-title example 45d

POST:

POST: plot

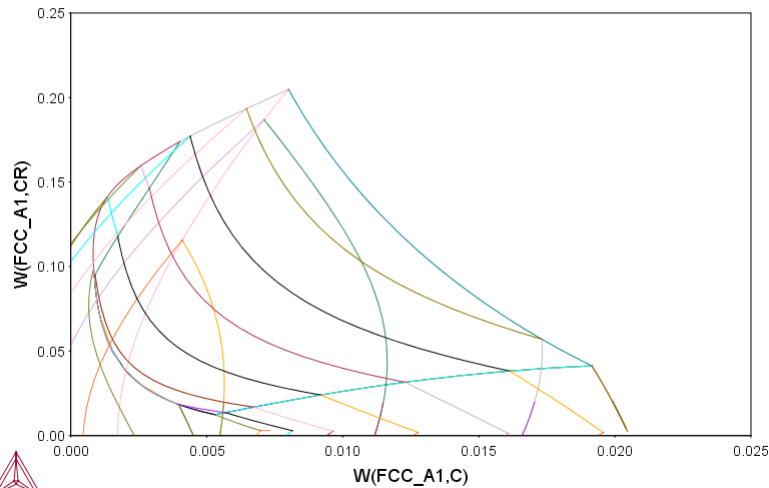
... the command in full is PLOT DIAGRAM

example 45d

2016.05.16.14.39.54

FEDEMO: C, CR, FE

N=1.,P=1E5



POST:

POST:

POST:Hit RETURN to continue

POST: @@ Enter the table for the calculated data.

POST: e-sym tab tabl

... the command in full is ENTER\_SYMBOL

Variable(s): W(fcc\_a1,c),W(fcc\_a1,cr),T;

POST:

POST: tab tabl fecrc.tab

... the command in full is TABULATE

POST:

POST: @@ Set the axis variables and the axis text for the final diagram

POST: s-a-t-s x n

... the command in full is SET\_AXIS\_TEXT\_STATUS

AXIS TEXT : Wei-Frac C

POST: s-a-t-s y n

... the command in full is SET\_AXIS\_TEXT\_STATUS

AXIS TEXT : Wei-Frac Cr

POST:

POST: s-d-a z temp-c

... the command in full is SET\_DIAGRAM\_AXIS

POST: s-a-t-s z n

... the command in full is SET\_AXIS\_TEXT\_STATUS

AXIS TEXT : Temp C

POST:

POST: @@ Finally, create the 3D-diagram (or .wrl file) by merging data

POST: @@ from the different tables created and saved. This is accomplished

POST: @@ using the command "CREATE\_3D\_DIAGRAM". Also define the scaling

POST: @@ to be used in the 3D-diagram.

POST: cre-3d

... the command in full is CREATE\_3D\_PLOTFILE

Use current WORKSPACE (WS), TAB files or BOTH: /WS/: BOTH

The table must contain values for X,Y and Z axis

DEFINED CONSTANTS

ZERO=0

DEFINED FUNCTIONS AND VARIABLES%

TEMP\_C=T-273.15

DEFINED TABLES

TAB1=W(FCC\_A1,C), W(FCC\_A1,CR), T

Table Name: tabl

Give TAB filename: /Cancel\_to\_finish/: fecr.tab fecrc.tab Cancel\_to\_finish

Output file: /3Dplot/: tcex45.wrl

X-AXIS SCALING FROM 0.0 TO XMAX /1/: .02

Y-AXIS SCALING FROM 0.0 TO YMAX /1/: .20

Z-AXIS SCALING, GIVE ZMIN /0/: 1000

Z-AXIS SCALING, GIVE ZMAX /2000/: 2000

It is possible to combine files by:

Copy Ter.tab+Bin1.tab+Bin2.tab+Bin3.tab Tmp.tab

Processing fecr.tab

3.5380900000000000E-010 <X> 2.0285100000000000E-002

0.0000000000000000E+000 <Y> 0.0000000000000000E+000

1011.180000000000 <Z> 1767.780000000000

Processing fecrc.tab

0.0000000000000000E+000 <X> 0.0000000000000000E+000

2.7415400000000000E-009 <Y> 0.1148050000000000

1126.340000000000 <Z> 1667.470000000000

POST:

POST:

POST: set-inter

... the command in full is SET\_INTERACTIVE\_MODE

POST:

## tcex46

About License library version: 8.5.1.0017  
Linked: Mon May 16 09:31:44 2016

```
SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex46\tcex46.TCM"SYS: set-echo
SYS: @@
SYS: @@ 3D-Diagram
SYS: @@ with the liquidus surface of the Fe-Cr-C system
SYS: @@
SYS: @@This file calculates the Liquidus surface in the FE-CR-C system
SYS: @@ Please note that in order to view the generated files, tcex46_tri.wrl
SYS: @@ and tcex46_sqrt, it's necessary to install a WRML(Virtual Reality
SYS: @@ Modelling Language) viewer to the web browser in use. WRML viwers
SYS: @@ can be downloaded from e.g. www.parallelgraphics.com and
SYS: @@ www.sim.no
SYS:
SYS: set-log ex46,,
SYS:
SYS: @@ Start by calculating the Fe-C side of the diagram
SYS: go data
... the command in full is GOTO_MODULE
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
L12_FCC          B2_BCC          B2_VACANCY
HIGH_SIGMA      DICTRA_FCC_A1   REJECTED

TDB_TCFE8: sw tcf7
... the command in full is SWITCH_DATABASE
Current database: Steels/Fe-Alloys v7.0

VA DEFINED
L12_FCC          B2_BCC          B2_VACANCY
HIGH_SIGMA      DICTRA_FCC_A1   REJECTED
TDB_TCFE7: de-sys fe c
... the command in full is DEFINE_SYSTEM
FE              C DEFINED
TDB_TCFE7: rej-ph * all
... the command in full is REJECT
GAS:G           LIQUID:L          BCC_A2
FCC_A1          HCP_A3           DIAMOND_FCC_A4
GRAPHITE        CEMENTITE        M23C6
M7C3           M5C2             KSI_CARBIDE
A1_KAPPA        KAPPA           FE4N_LP1
FECN_CHI        LAVES_PHASE_C14 REJECTED
TDB_TCFE7: res-ph fcc_a1,bcc_a2,cementite,graphite,liquid
... the command in full is RESTORE
FCC_A1          BCC_A2           CEMENTITE
GRAPHITE        LIQUID:L        RESTORED
TDB_TCFE7: get
... the command in full is GET_DATA
REINITIATING GES5 .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
-FE'
'B. Uhrenius (1993-1994), International journal of refractory metals and
hard mater, Vol. 12, pp. 121-127; Molar volumes'
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
Molar volumes'
'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
-OK-
TDB_TCFE7:
TDB_TCFE7: go poly
... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3: s-c t=1973
... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
... the command in full is SET_CONDITION
POLY_3: se-co x(c)=2e-2
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated          413 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution          0 s, total time          0 s
POLY_3: s-a-v 1 x(c) 0 1 .01
... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 t 1300 5000 20
... the command in full is SET_AXIS_VARIABLE
POLY_3: advanced
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /NONE/: liq
POLY_3:
POLY_3: save tcex46 y
... the command in full is SAVE_WORKSPACES
POLY_3: map
Version S mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
```



Generating start equilibrium 10  
Generating start equilibrium 11  
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1  
Generating start point 2  
Generating start point 3  
Generating start point 4  
Generating start point 5  
Generating start point 6  
Generating start point 7  
Generating start point 8  
Generating start point 9  
Generating start point 10

Working hard

Generating start point 11  
Generating start point 12  
Generating start point 13  
Generating start point 14  
Generating start point 15  
Generating start point 16  
Generating start point 17  
Generating start point 18  
Generating start point 19  
Generating start point 20

Working hard

Generating start point 21  
Generating start point 22  
Generating start point 23  
Generating start point 24  
Generating start point 25  
Generating start point 26  
Generating start point 27  
Generating start point 28

Phase region boundary 1 at: 1.982E-02 1.759E+03

\*\* LIQUID

FCC\_A1

Calculated. 2 equilibria

Phase region boundary 2 at: 1.599E-02 1.768E+03

\*\* LIQUID

\*\* BCC\_A2

FCC\_A1

Phase region boundary 3 at: 1.417E-02 1.768E+03

LIQUID

\*\* BCC\_A2

Calculated 15 equilibria

Phase region boundary 4 at: 1.599E-02 1.768E+03

\*\* LIQUID

FCC\_A1

Calculated. 19 equilibria

Phase region boundary 5 at: 1.310E-01 1.427E+03

\*\* LIQUID

FCC\_A1

\*\* GRAPHITE

Phase region boundary 6 at: 5.871E-01 1.427E+03

LIQUID

\*\* GRAPHITE

Calculated 178 equilibria

Phase region boundary 7 at: 1.982E-02 1.759E+03

\*\* LIQUID

FCC\_A1

Calculated. 24 equilibria

Terminating at known equilibrium

Phase region boundary 8 at: 6.344E-01 2.537E+03

LIQUID

\*\* GRAPHITE

Calculated. 57 equilibria

Terminating at known equilibrium

Phase region boundary 9 at: 6.344E-01 2.537E+03

LIQUID

\*\* GRAPHITE

Calculated 128 equilibria

Phase region boundary 10 at: 6.344E-01 2.537E+03

LIQUID

\*\* GRAPHITE

Calculated. 57 equilibria

Terminating at known equilibrium

Phase region boundary 11 at: 6.344E-01 2.537E+03

LIQUID

\*\* GRAPHITE

Calculated 128 equilibria

Phase region boundary 12 at: 7.226E-01 3.763E+03

LIQUID

\*\* GRAPHITE

Calculated. 118 equilibria

Terminating at known equilibrium

Phase region boundary 13 at: 7.226E-01 3.763E+03

LIQUID

\*\* GRAPHITE

Calculated 64 equilibria

Phase region boundary 14 at: 7.226E-01 3.763E+03

LIQUID

\*\* GRAPHITE

Calculated. 118 equilibria

Terminating at known equilibrium

Phase region boundary 15 at: 7.226E-01 3.763E+03

LIQUID

```

** GRAPHITE
Calculated                      64 equilibria

Phase region boundary 16 at:    5.888E-03  1.794E+03
LIQUID
** BCC_A2
Calculated                      13 equilibria

Phase region boundary 17 at:    5.888E-03  1.794E+03
LIQUID
** BCC_A2
Calculated.                      3 equilibria
Terminating at known equilibrium

Phase region boundary 18 at:    6.683E-01  3.181E+03
LIQUID
** GRAPHITE
Calculated.                      89 equilibria
Terminating at known equilibrium

Phase region boundary 19 at:    6.683E-01  3.181E+03
LIQUID
** GRAPHITE
Calculated                      92 equilibria

Phase region boundary 20 at:    8.317E-01  4.174E+03
LIQUID
** GRAPHITE
Calculated.                     147 equilibria
Terminating at known equilibrium

Phase region boundary 21 at:    8.317E-01  4.174E+03
LIQUID
** GRAPHITE
Calculated                      43 equilibria

Phase region boundary 22 at:    9.950E-01  4.749E+03
LIQUID
** GRAPHITE
Calculated.                     179 equilibria
Terminating at known equilibrium

Phase region boundary 23 at:    9.950E-01  4.749E+03
LIQUID
** GRAPHITE
Calculated                      18 equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex46\tcex
46.POLY3
CPU time for mapping                      1 seconds
POLY_3:
POLY_3: post

```

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

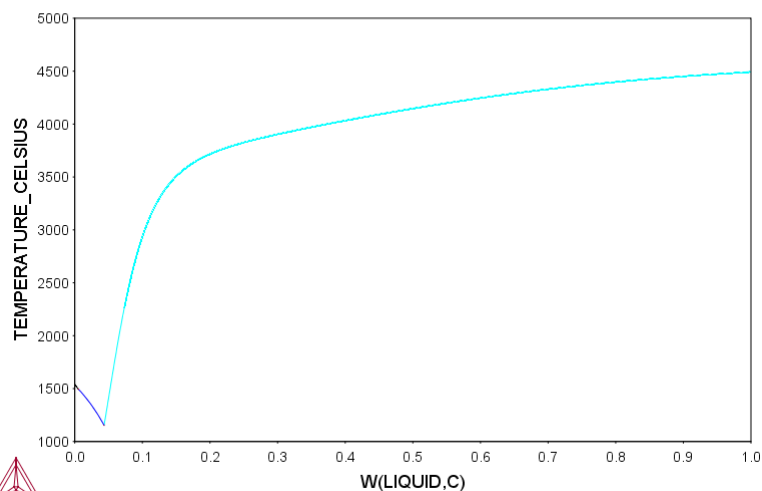
```

POST: s-d-a x w(liquid,c)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y te-c
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 46a
POST: plot
... the command in full is PLOT DIAGRAM

```

**example 46a**

2016.05.16.14.42.12  
TCFE7: C,FE  
N=1,P=1E5



```

POST:
POST:
POST: Hit RETURN to continue
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the C content in the liquid, in the second the Cr content,
POST: @@ and in the last column the temperature.
POST: e-sym tab tab1
... the command in full is ENTER_SYMBOL
Variable(s): W(liquid,c),zero,Temp_c
&
POST: @@ Save the tabulated data on file
POST: tab tab1 fec_liq.tab
... the command in full is TABULATE
POST: back
POLY_3:
POLY_3: @@ Next calculate the Fe-Cr side of the diagram

```

```

POLY_3: go data
... the command in full is GOTO_MODULE
TDB_TCFE7: rej-sys
... the command in full is REJECT
VA DEFINED
L12_FCC B2_BCC B2_VACANCY
HIGH_SIGMA DICTRA_FCC_A1 REJECTED
REINITIATING GES5 .....
TDB_TCFE7: de-sys fe cr
... the command in full is DEFINE_SYSTEM
FE CR DEFINED
TDB_TCFE7: rej-ph * all
... the command in full is REJECT
LIQUID:L BCC_A2 FCC_A1
HCP_A3 A1_KAPPA KAPPA
SIGMA CHI_A12 LAVES_PHASE_C14
CR3SI REJECTED
TDB_TCFE7: res-ph bcc_a2,liquid
... the command in full is RESTORE
BCC_A2 LIQUID:L RESTORED
TDB_TCFE7: get
... the command in full is GET_DATA
REINITIATING GES5 .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ...

List of references for assessed data

'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
'B.-J. Lee, Calphad (1993); revision of Fe-Cr and Fe-Ni liquid'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
Molar volumes'
'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
'J.-O. Andersson and B. Sundman, Calphad, 11 (1987), 83-92; TRITA 0270
(1986); CR-FE'
-OK-
TDB_TCFE7:
TDB_TCFE7: go poly
... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3: s-c t=2373
... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
... the command in full is SET_CONDITION
POLY_3: se-co x(cr)=2e-2
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 274 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY_3: s-a-v 1 x(cr) 0 1 .01
... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 t 1500 2400 10
... the command in full is SET_AXIS_VARIABLE
POLY_3: advanced
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /NONE/: liquid
POLY_3:
POLY_3: save tcex46 y
... the command in full is SAVE_WORKSPACES

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

POLY_3:
POLY_3: map
Version 8 mapping is selected
Generating start equilibrium 1
Generating start equilibrium 2
Generating start equilibrium 3
Generating start equilibrium 4
Generating start equilibrium 5
Generating start equilibrium 6
Generating start equilibrium 7
Generating start equilibrium 8
Generating start equilibrium 9
Generating start equilibrium 10
Generating start equilibrium 11
Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20

```

Working hard  
Generating start point 21  
Generating start point 22  
Generating start point 23  
Generating start point 24

Phase region boundary 1 at: 1.039E-02 1.809E+03  
\*\* LIQUID  
BCC\_A2  
Calculated 14 equilibria

Phase region boundary 2 at: 1.039E-02 1.809E+03  
\*\* LIQUID  
BCC\_A2  
Calculated 110 equilibria

Phase region boundary 3 at: 3.280E-01 1.802E+03  
\*\* LIQUID  
BCC\_A2  
Calculated 43 equilibria

Phase region boundary 4 at: 3.280E-01 1.802E+03  
\*\* LIQUID  
BCC\_A2  
Calculated 81 equilibria

Phase region boundary 5 at: 6.371E-01 1.971E+03  
\*\* LIQUID  
BCC\_A2  
Calculated 76 equilibria

Phase region boundary 6 at: 6.371E-01 1.971E+03  
\*\* LIQUID  
BCC\_A2  
Calculated 48 equilibria

Phase region boundary 7 at: 9.888E-01 2.175E+03  
\*\* LIQUID  
BCC\_A2  
Calculated 114 equilibria

Phase region boundary 8 at: 9.888E-01 2.175E+03  
\*\* LIQUID  
BCC\_A2  
Calculated 10 equilibria

Phase region boundary 9 at: 5.100E-02 1.803E+03  
\*\* LIQUID  
BCC\_A2  
Calculated 105 equilibria

Phase region boundary 10 at: 5.100E-02 1.803E+03  
\*\* LIQUID  
BCC\_A2  
Calculated 12 equilibria

Phase region boundary 11 at: 3.337E-01 1.803E+03  
\*\* LIQUID  
BCC\_A2  
Calculated 44 equilibria

Phase region boundary 12 at: 3.337E-01 1.803E+03  
\*\* LIQUID  
BCC\_A2  
Calculated 102 equilibria

Phase region boundary 13 at: 8.293E-01 2.097E+03  
LIQUID  
\*\* BCC\_A2  
Calculated 111 equilibria

Phase region boundary 14 at: 8.293E-01 2.097E+03  
LIQUID  
\*\* BCC\_A2  
Calculated 32 equilibria

Phase region boundary 15 at: 8.293E-01 2.097E+03  
\*\* LIQUID  
BCC\_A2  
Calculated 111 equilibria

Phase region boundary 16 at: 8.293E-01 2.097E+03  
\*\* LIQUID  
BCC\_A2  
Calculated 32 equilibria

Phase region boundary 17 at: 9.640E-03 1.809E+03  
LIQUID  
\*\* BCC\_A2  
Calculated 15 equilibria

Phase region boundary 18 at: 9.640E-03 1.809E+03  
LIQUID  
\*\* BCC\_A2  
Calculated 109 equilibria

Phase region boundary 19 at: 3.471E-01 1.807E+03  
LIQUID  
\*\* BCC\_A2  
Calculated 49 equilibria

Phase region boundary 20 at: 3.471E-01 1.807E+03  
LIQUID  
\*\* BCC\_A2  
Calculated 75 equilibria

Phase region boundary 21 at: 6.881E-01 2.007E+03  
LIQUID  
\*\* BCC\_A2  
Calculated 83 equilibria

Phase region boundary 22 at: 6.881E-01 2.007E+03  
LIQUID  
\*\* BCC\_A2  
Calculated 41 equilibria

```

Phase region boundary 23 at: 9.910E-01 2.176E+03
LIQUID
** BCC_A2
Calculated 106 equilibria

Phase region boundary 24 at: 9.910E-01 2.176E+03
LIQUID
** BCC_A2
Calculated 14 equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex46\tcex
46.POLY3
CPU time for mapping 1 seconds
POLY_3:
POLY_3: post

```

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

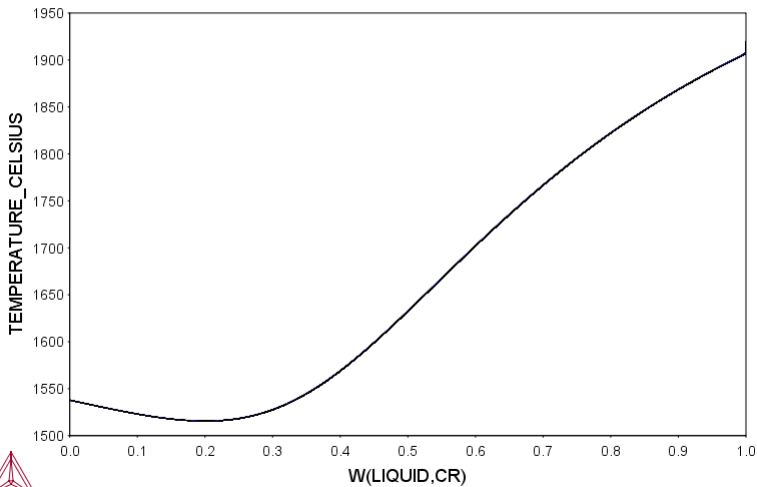
```

POST: s-d-a x W(liquid,cr)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y te-c
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 46b
POST:
POST: plot
... the command in full is PLOT DIAGRAM

```

example 46b

2016.05.16.14.42.23  
TCFE7:CR,FE  
N=1,P=1E5



```

POST:
POST:
POST:Hit RETURN to continue
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the C content in the liquid, in the second the Cr content,
POST: @@ and in the last column the temperature.
POST: e-sym tab tab1
... the command in full is ENTER_SYMBOL
Variable(s): zero,W(liquid,cr),Temp_c
&
POST: @@ Save the tabulated data on file
POST: tab tab1 fccr_liq.tab
... the command in full is TABULATE
POST: back
POLY_3:
POLY_3: @@ Then calculate the Cr-C side of the diagram
POLY_3: go data
... the command in full is GOTO_MODULE
TDB_TCFE7: rej-sys
... the command in full is REJECT
VA DEFINED
LI2_FCC B2_BCC B2_VACANCY
HIGH_SIGMA DICTRA_FCC_A1 REJECTED
REINITIATING GES5 .....
TDB_TCFE7: de-sys c cr
... the command in full is DEFINE_SYSTEM
C CR DEFINED
TDB_TCFE7: rej-ph * all
... the command in full is REJECT
GAS:G LIQUID:L BCC_A2
FCC_A1 HCP_A3 DIAMOND_FCC_A4
GRAPHITE CEMENTITE M23C6
M7C3 M3C2 KSI_CARBIDE
FE4N_LP1 SIGMA CHI_A12
LAVES_PHASE_C14 CR3SI REJECTED
TDB_TCFE7: res-ph bcc_a2,liquid,graphite,m23,m7c,m3c2
... the command in full is RESTORE
BCC_A2 LIQUID:L GRAPHITE
M23C6 M7C3 M3C2
RESTORED
TDB_TCFE7: get
... the command in full is GET_DATA
REINITIATING GES5 .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

```

List of references for assessed data

'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'  
 'J-O. Andersson, Calphad, 11 (1987), 271-276; TRITA 0314; C-CR'  
 'B. Uhrenius (1993-1994), International journal of refractory metals and hard mater, Vol. 12, pp. 121-127; Molar volumes'  
 'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'  
 'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89; Molar volumes'  
 'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'  
 'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'  
 'P. Villars and L.D. Calvert (1985). Pearsons handbook of crystallographic data for intermetallic phases. Metals park, Ohio. American Society for Metals; Molar volumes'

-OK-

**TDB\_TCFE7:**

**TDB\_TCFE7:** go poly

... the command in full is GOTO\_MODULE

POLY version 3.32

**POLY\_3:** s-c t=2373

... the command in full is SET\_CONDITION

**POLY\_3:** se-co n=1,p=1e5

... the command in full is SET\_CONDITION

**POLY\_3:** se-co x(cr)=1.5e-2

... the command in full is SET\_CONDITION

**POLY\_3:** c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Using global minimization procedure

Calculated 278 grid points in 0 s

Found the set of lowest grid points in 0 s

Calculated POLY solution 0 s, total time 0 s

**POLY\_3:** s-a-v 1 x(cr) 0 1 .01

... the command in full is SET\_AXIS\_VARIABLE

**POLY\_3:** s-a-v 2 t 1500 5000 10

... the command in full is SET\_AXIS\_VARIABLE

**POLY\_3:** advanced

... the command in full is ADVANCED\_OPTIONS

**Which option? /STEP\_AND\_MAP/:** present

**Phase name /NONE/:** liq

**POLY\_3:**

**POLY\_3:** save tcex46 y

... the command in full is SAVE\_WORKSPACES

This file contains results from a previous STEP or MAP command.

The SAVE command will save the current status of the program but destroy

the results from the previous STEP or MAP commands.

**POLY\_3:**

**POLY\_3:** map

Version 3 mapping is selected

Generating start equilibrium 1

Generating start equilibrium 2

Generating start equilibrium 3

Generating start equilibrium 4

Generating start equilibrium 5

Generating start equilibrium 6

Generating start equilibrium 7

Generating start equilibrium 8

Generating start equilibrium 9

Generating start equilibrium 10

Generating start equilibrium 11

Generating start equilibrium 12

Organizing start points

Using ADDED start equilibria

Generating start point 1

Generating start point 2

Generating start point 3

Generating start point 4

Generating start point 5

Generating start point 6

Generating start point 7

Generating start point 8

Generating start point 9

Generating start point 10

Working hard

Generating start point 11

Generating start point 12

Generating start point 13

Generating start point 14

Generating start point 15

Generating start point 16

Generating start point 17

Generating start point 18

Generating start point 19

Generating start point 20

Working hard

Generating start point 21

Generating start point 22

Generating start point 23

Generating start point 24

Generating start point 25

Generating start point 26

Generating start point 27

Generating start point 28

Phase region boundary 1 at: 2.762E-01 2.670E+03

LIQUID

\*\* GRAPHITE

Calculated. 61 equilibria

Phase region boundary 2 at: 3.108E-01 2.077E+03

LIQUID

\*\* GRAPHITE

\*\* M3C2

Phase region boundary 3 at: 6.108E-01 2.077E+03

LIQUID

\*\* M3C2

Calculated. 7 equilibria

Phase region boundary 4 at: 6.354E-01 2.018E+03

LIQUID

\*\* M3C2

```

** M7C3
Phase region boundary 5 at: 6.854E-01 2.018E+03
LIQUID
** M7C3
Calculated. 36 equilibria
Phase region boundary 6 at: 7.604E-01 1.850E+03
LIQUID
** M23C6
** M7C3
Phase region boundary 7 at: 8.070E-01 1.850E+03
LIQUID
** M23C6
Calculated. 6 equilibria
Phase region boundary 8 at: 8.281E-01 1.806E+03
LIQUID
** BCC_A2
** M23C6
Phase region boundary 9 at: 9.300E-01 1.806E+03
LIQUID
** BCC_A2
Calculated 54 equilibria
Phase region boundary 10 at: 3.108E-01 2.077E+03
LIQUID
** GRAPHITE
Calculated 289 equilibria
Phase region boundary 11 at: 2.762E-01 2.670E+03
LIQUID
** GRAPHITE
Calculated 222 equilibria
Phase region boundary 12 at: 2.762E-01 2.670E+03
LIQUID
** GRAPHITE
Calculated. 61 equilibria
Terminating at known equilibrium
Phase region boundary 13 at: 2.762E-01 2.670E+03
LIQUID
** GRAPHITE
Calculated 222 equilibria
Phase region boundary 14 at: 2.023E-01 3.830E+03
LIQUID
** GRAPHITE
Calculated. 177 equilibria
Terminating at known equilibrium
Phase region boundary 15 at: 2.023E-01 3.830E+03
LIQUID
** GRAPHITE
Calculated 106 equilibria
Phase region boundary 16 at: 2.023E-01 3.830E+03
LIQUID
** GRAPHITE
Calculated. 177 equilibria
Terminating at known equilibrium
Phase region boundary 17 at: 2.023E-01 3.830E+03
LIQUID
** GRAPHITE
Calculated 106 equilibria
Phase region boundary 18 at: 5.000E-03 4.751E+03
LIQUID
** GRAPHITE
Calculated 18 equilibria
Phase region boundary 19 at: 5.000E-03 4.751E+03
LIQUID
** GRAPHITE
Calculated. 276 equilibria
Terminating at known equilibrium
Phase region boundary 20 at: 1.683E-01 4.226E+03
LIQUID
** GRAPHITE
Calculated 73 equilibria
Phase region boundary 21 at: 1.683E-01 4.226E+03
LIQUID
** GRAPHITE
Calculated. 216 equilibria
Terminating at known equilibrium
Phase region boundary 22 at: 6.317E-01 2.031E+03
LIQUID
** M3C2
Calculated. 7 equilibria
Terminating at known equilibrium
Phase region boundary 23 at: 6.317E-01 2.031E+03
LIQUID
** M3C2
Calculated. 3 equilibria
Terminating at known equilibrium
Phase region boundary 24 at: 9.949E-01 2.162E+03
LIQUID
** BCC_A2
Calculated. 38 equilibria
Terminating at known equilibrium
Phase region boundary 25 at: 9.949E-01 2.162E+03
LIQUID
** BCC_A2
Calculated 14 equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex46\tcex

```

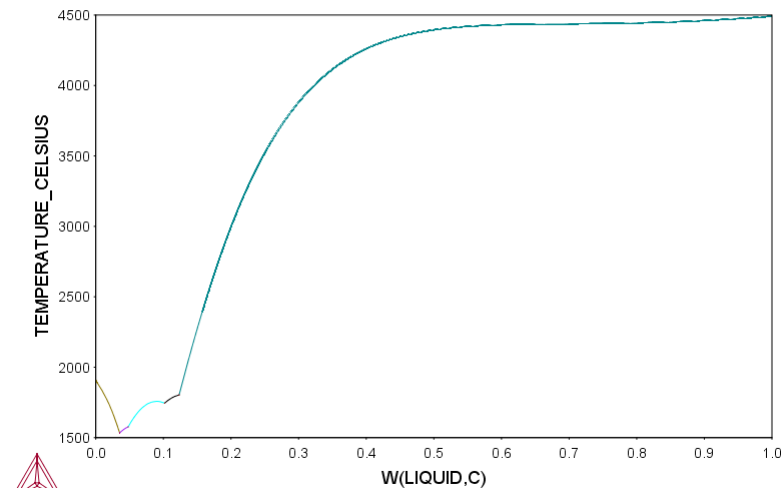
```
46.POLY3
CPU time for mapping          1 seconds
POLY_3:
POLY_3: post
```

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

```
POST: s-d-a x w(liquid,C)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y temp-c
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 46c
POST:
POST: plot
... the command in full is PLOT DIAGRAM
                                example 46c
```

2016.05.16.14.42.34  
TCFE7: C, CR  
N=1, P=1E5



```
POST:
POST:
POST: Hit RETURN to continue
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the C content in the liquid, in the second the Cr content,
POST: @@ and in the last column the temperature.
POST: e-sym tab tabl
... the command in full is ENTER_SYMBOL
Variable(s): W(liquid,c),W(liquid,cr),Temp_c
&
POST: @@ Save the tabulated data on file
POST: tab tabl crc_liq.tab
... the command in full is TABULATE
POST:
POST: back
POLY_3: @@ Finally, calculate a ternary projection of the Fe-Cr-C system
POLY_3: go data
... the command in full is GOTO_MODULE
TDB_TCFE7: rej-sys
... the command in full is REJECT
VA DEFINED
L12 FCC          B2_BCC          B2_VACANCY
HIGH_SIGMA      DICTRA_FCC_A1   REJECTED
REINITIATING GES5 .....
TDB_TCFE7: de-sys fe cr c
... the command in full is DEFINE_SYSTEM
FE          CR          C
DEFINED
TDB_TCFE7: rej-ph * all
... the command in full is REJECT
GAS:G          LIQUID:L          BCC_A2
FCC_A1          HCP_A3          DIAMOND_FCC_A4
GRAPHITE        CEMENTITE        M23C6
M7C3            M5C2            M3C2
KSI CARBIDE     A1 KAPPA          KAPPA
FE4N LP1        FECN_CHI          SIGMA
CHI A12         LAVES_PHASE_C14   CR3SI
REJECTED
TDB_TCFE7: res-ph liquid,fcc_a1,bcc_a2,m23,m7c,m3c2,graphite,cementite
... the command in full is RESTORE
LIQUID:L        FCC_A1          BCC_A2
M23C6           M7C3            M3C2
GRAPHITE        CEMENTITE       RESTORED
TDB_TCFE7: get
... the command in full is GET_DATA
REINITIATING GES5 .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....
```

List of references for assessed data

'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'  
'J-O. Andersson, Calphad, 11 (1987), 271-276; TRITA 0314; C-CR'  
'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C-  
-FE'  
'B.-J. Lee, Calphad (1993); revision of Fe-Cr and Fe-Ni liquid'  
'B. Uhrenius (1993-1994), International journal of refractory metals and  
hard mater, Vol. 12, pp. 121-127; Molar volumes'



'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'  
 'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;  
 Molar volumes'  
 'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'  
 'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'  
 'J.-O. Andersson and B. Sundman, Calphad, 11 (1987), 83-92; TRITA 0270  
 (1986); CR-FE'  
 'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'  
 'J.-O. Andersson, Metall. Trans. A, 19A (1988), 627-636 TRITA 0207 (1986);  
 C-CR-FE'  
 'J. Bratberg, Z. Metallkd., Vol 96 (2005), 335-344; Fe-Cr-Mo-C'  
 'P. Villars and L.D. Calvert (1985). Pearsons handbook of crystallographic  
 data for intermetallic phases. Metals park, Ohio. American Society for  
 Metals; Molar volumes'

-OK-

**TDB\_TCFE7:**

**TDB\_TCFE7:** go poly

... the command in full is GOTO\_MODULE

POLY version 3.32

**POLY\_3:** s-c t=1373

... the command in full is SET\_CONDITION

**POLY\_3:** se-co n=1,p=1e5

... the command in full is SET\_CONDITION

**POLY\_3:** se-co x(c)=.01

... the command in full is SET\_CONDITION

**POLY\_3:** se-co x(cr)=2e-2

... the command in full is SET\_CONDITION

**POLY\_3:** c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Using global minimization procedure

Calculated 7710 grid points in 0 s

Found the set of lowest grid points in 0 s

Calculated POLY solution 0 s, total time 0 s

**POLY\_3:**

**POLY\_3:** s-a-v 1 x(c) 0 1 .01

... the command in full is SET\_AXIS\_VARIABLE

**POLY\_3:** s-a-v 2 x(cr) 0 1 .01

... the command in full is SET\_AXIS\_VARIABLE

**POLY\_3:**

**POLY\_3:** se-con t=1600

... the command in full is SET\_CONDITION

**POLY\_3:** c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Using global minimization procedure

Calculated 7710 grid points in 0 s

Found the set of lowest grid points in 0 s

Calculated POLY solution 0 s, total time 0 s

**POLY\_3:** add-in 1

... the command in full is ADD\_INITIAL\_EQUILIBRIUM

**POLY\_3:**

**POLY\_3:** se-con t=1700

... the command in full is SET\_CONDITION

**POLY\_3:** c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Using global minimization procedure

Calculated 7710 grid points in 0 s

Found the set of lowest grid points in 0 s

Calculated POLY solution 0 s, total time 0 s

**POLY\_3:** add-in 1

... the command in full is ADD\_INITIAL\_EQUILIBRIUM

**POLY\_3:**

**POLY\_3:** se-con t=1800

... the command in full is SET\_CONDITION

**POLY\_3:** c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Using global minimization procedure

Calculated 7710 grid points in 0 s

Found the set of lowest grid points in 0 s

Calculated POLY solution 0 s, total time 0 s

**POLY\_3:** add-in 1

... the command in full is ADD\_INITIAL\_EQUILIBRIUM

**POLY\_3:**

**POLY\_3:** se-con t=1900

... the command in full is SET\_CONDITION

**POLY\_3:** c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Using global minimization procedure

Calculated 7710 grid points in 0 s

Found the set of lowest grid points in 0 s

Calculated POLY solution 0 s, total time 0 s

**POLY\_3:** add-in 1

... the command in full is ADD\_INITIAL\_EQUILIBRIUM

**POLY\_3:**

**POLY\_3:** se-con t=2000

... the command in full is SET\_CONDITION

**POLY\_3:** c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Using global minimization procedure

Calculated 7710 grid points in 0 s

Found the set of lowest grid points in 0 s

Calculated POLY solution 0 s, total time 0 s

**POLY\_3:** add-in 1

... the command in full is ADD\_INITIAL\_EQUILIBRIUM

**POLY\_3:**

**POLY\_3:** se-con t=2100

... the command in full is SET\_CONDITION

**POLY\_3:** c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Using global minimization procedure

Calculated 7710 grid points in 0 s

Found the set of lowest grid points in 0 s

Calculated POLY solution 0 s, total time 0 s

**POLY\_3:** add-in 1

... the command in full is ADD\_INITIAL\_EQUILIBRIUM

**POLY\_3:**

**POLY\_3:** se-con t=2200

... the command in full is SET\_CONDITION

**POLY\_3:** c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Using global minimization procedure

Calculated 7710 grid points in 0 s

Found the set of lowest grid points in 0 s

Calculated POLY solution 0 s, total time 0 s

```

POLY_3: add-in 1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-co x(c)=.01
... the command in full is SET_CONDITION
POLY_3: se-co x(cr)=9e-2
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Using already calculated grid
Found the set of lowest grid points in          0 s
Calculated POLY solution          0 s, total time    0 s
POLY_3:
POLY_3: se-con t=1900
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated          7710 grid points in          1 s
Found the set of lowest grid points in          0 s
Calculated POLY solution          0 s, total time    1 s
POLY_3: add-in 2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=2000
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated          7710 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution          0 s, total time    0 s
POLY_3: add-in 2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-con t=2100
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated          7710 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution          0 s, total time    0 s
POLY_3: add-in 2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: advanced
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /NONE/: liq
POLY_3:
POLY_3: save fecrc y
... the command in full is SAVE_WORKSPACES
POLY_3:
POLY_3: map
Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point  1
Generating start point  2
Generating start point  3
Generating start point  4
Generating start point  5
Generating start point  6
Generating start point  7
Generating start point  8
Generating start point  9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard

Phase region boundary  1 at:   8.271E-02  2.328E-02
** LIQUID
FCC_A1
Calculated.          11 equilibria

Phase region boundary  2 at:   8.271E-02  2.328E-02
** LIQUID
FCC_A1
Calculated.          23 equilibria

Phase region boundary  3 at:   6.085E-02  2.377E-01
** LIQUID
** BCC_A2
FCC_A1

Phase region boundary  4 at:   4.944E-02  2.509E-01
LIQUID
** BCC_A2
Calculated.          22 equilibria

Phase region boundary  5 at:   5.504E-02  4.549E-01
LIQUID
** BCC_A2
** M23C6

Phase region boundary  6 at:   1.550E-01  5.383E-01
LIQUID
** M23C6
Calculated.          3 equilibria

```

Phase region boundary 7 at: 1.594E-01 5.202E-01  
LIQUID  
\*\* M23C6  
\*\* M7C3

Phase region boundary 8 at: 2.060E-01 5.178E-01  
LIQUID  
\*\* M7C3  
Calculated. 38 equilibria

Phase region boundary 9 at: 2.657E-01 1.556E-01  
LIQUID  
\*\* GRAPHITE  
\*\* M7C3

Phase region boundary 10 at: 6.157E-01 4.922E-02  
LIQUID  
\*\* GRAPHITE  
Calculated 18 equilibria

Phase region boundary 11 at: 6.085E-02 2.377E-01  
\*\* LIQUID  
FCC\_A1  
Calculated 35 equilibria

Phase region boundary 12 at: 4.494E-02 2.178E-02  
\*\* LIQUID  
FCC\_A1  
Calculated 16 equilibria

Phase region boundary 13 at: 4.494E-02 2.178E-02  
\*\* LIQUID  
FCC\_A1  
Calculated. 13 equilibria

Phase region boundary 14 at: 3.129E-02 1.383E-01  
\*\* LIQUID  
\*\* BCC\_A2  
FCC\_A1

Phase region boundary 15 at: 2.528E-02 1.443E-01  
LIQUID  
\*\* BCC\_A2  
Calculated. 59 equilibria

Phase region boundary 16 at: 6.178E-02 7.198E-01  
LIQUID  
\*\* BCC\_A2  
\*\* M23C6

Phase region boundary 17 at: 1.633E-01 7.006E-01  
LIQUID  
\*\* M23C6  
Calculated. 7 equilibria

Phase region boundary 18 at: 1.771E-01 6.455E-01  
LIQUID  
\*\* M23C6  
\*\* M7C3

Phase region boundary 19 at: 2.237E-01 6.202E-01  
LIQUID  
\*\* M7C3  
Calculated. 40 equilibria

Phase region boundary 20 at: 2.886E-01 2.325E-01  
LIQUID  
\*\* GRAPHITE  
\*\* M7C3

Phase region boundary 21 at: 6.386E-01 9.541E-02  
LIQUID  
\*\* GRAPHITE  
Calculated 29 equilibria

Phase region boundary 22 at: 3.129E-02 1.383E-01  
\*\* LIQUID  
FCC\_A1  
Calculated 28 equilibria

Phase region boundary 23 at: 6.080E-01 1.000E-02  
LIQUID  
\*\* GRAPHITE  
Calculated 22 equilibria

Phase region boundary 24 at: 6.080E-01 1.000E-02  
LIQUID  
\*\* GRAPHITE  
Calculated. 30 equilibria

Phase region boundary 25 at: 6.645E-01 1.791E-01  
LIQUID  
\*\* GRAPHITE  
\*\* M7C3

Phase region boundary 26 at: 3.145E-01 3.964E-01  
LIQUID  
\*\* M7C3  
Calculated. 53 equilibria

Phase region boundary 27 at: 2.351E-01 7.127E-01  
LIQUID  
\*\* M23C6  
\*\* M7C3

Phase region boundary 28 at: 1.885E-01 7.542E-01  
LIQUID  
\*\* M23C6  
Calculated. 8 equilibria

Phase region boundary 29 at: 1.714E-01 8.208E-01  
LIQUID  
\*\* BCC\_A2  
\*\* M23C6

Phase region boundary 30 at: 6.952E-02 9.185E-01  
 LIQUID  
 \*\* BCC\_A2  
 Calculated 80 equilibria

Phase region boundary 31 at: 6.645E-01 1.791E-01  
 LIQUID  
 \*\* GRAPHITE  
 Calculated 42 equilibria

Phase region boundary 32 at: 6.125E-01 1.000E-02  
 LIQUID  
 \*\* GRAPHITE  
 Calculated 6 equilibria

Phase region boundary 33 at: 6.125E-01 1.000E-02  
 LIQUID  
 \*\* GRAPHITE  
 Calculated. 37 equilibria

Phase region boundary 34 at: 6.771E-01 2.438E-01  
 LIQUID  
 \*\* GRAPHITE  
 \*\* M3C2

Phase region boundary 35 at: 3.771E-01 5.438E-01  
 LIQUID  
 \*\* M3C2  
 Calculated. 2 equilibria

Phase region boundary 36 at: 3.711E-01 5.535E-01  
 LIQUID  
 \*\* M3C2  
 \*\* M7C3

Phase region boundary 37 at: 3.211E-01 5.530E-01  
 LIQUID  
 \*\* M7C3  
 Calculated 52 equilibria

Phase region boundary 38 at: 6.771E-01 2.438E-01  
 LIQUID  
 \*\* GRAPHITE  
 Calculated 48 equilibria

Phase region boundary 39 at: 6.169E-01 1.000E-02  
 LIQUID  
 \*\* GRAPHITE  
 Calculated 6 equilibria

Phase region boundary 40 at: 6.169E-01 1.000E-02  
 LIQUID  
 \*\* GRAPHITE  
 Calculated. 40 equilibria

Phase region boundary 41 at: 6.845E-01 2.766E-01  
 LIQUID  
 \*\* GRAPHITE  
 \*\* M3C2

Phase region boundary 42 at: 3.845E-01 5.766E-01  
 LIQUID  
 \*\* M3C2  
 Calculated. 6 equilibria

Phase region boundary 43 at: 3.652E-01 6.202E-01  
 LIQUID  
 \*\* M3C2  
 \*\* M7C3

Phase region boundary 44 at: 3.152E-01 6.637E-01  
 LIQUID  
 \*\* M7C3  
 Calculated 37 equilibria

Phase region boundary 45 at: 6.845E-01 2.766E-01  
 LIQUID  
 \*\* GRAPHITE  
 Calculated 55 equilibria

Phase region boundary 46 at: 6.214E-01 1.000E-02  
 LIQUID  
 \*\* GRAPHITE  
 Calculated 22 equilibria

Phase region boundary 47 at: 6.214E-01 1.000E-02  
 LIQUID  
 \*\* GRAPHITE  
 Calculated 66 equilibria

Phase region boundary 48 at: 6.259E-01 1.000E-02  
 LIQUID  
 \*\* GRAPHITE  
 Calculated 22 equilibria

Phase region boundary 49 at: 6.259E-01 1.000E-02  
 LIQUID  
 \*\* GRAPHITE  
 Calculated 62 equilibria

Phase region boundary 50 at: 5.307E-03 5.782E-01  
 LIQUID  
 \*\* BCC\_A2  
 Calculated 26 equilibria

Phase region boundary 51 at: 5.307E-03 5.782E-01  
 LIQUID  
 \*\* BCC\_A2  
 Calculated 54 equilibria

Phase region boundary 52 at: 5.190E-03 7.168E-01  
 LIQUID  
 \*\* BCC\_A2  
 Calculated 20 equilibria

Phase region boundary 53 at: 5.190E-03 7.168E-01

```

    LIQUID
** BCC_A2
Calculated                      40 equilibria

Phase region boundary 54 at:    5.138E-03  8.727E-01
    LIQUID
** BCC_A2
Calculated                      26 equilibria

Phase region boundary 55 at:    5.138E-03  8.727E-01
    LIQUID
** BCC_A2
Calculated                      30 equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex46\fecr
c.POLY3
CPU time for mapping              4 seconds
POLY_3:
POLY_3: s-a-v 1 x(c) 0 1 .01
... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(cr) 0 1 .01
... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 3 T 1000 3000 8
... the command in full is SET_AXIS_VARIABLE
POLY_3: se-con x(cr)=.6
... the command in full is SET_CONDITION
POLY_3: se-con x(c)=.01
... the command in full is SET_CONDITION
POLY_3: se-con t=1873
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated                      7710 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution          0 s, total time          0 s
POLY_3: ad-ini 1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: advanced
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /LIQUID#1/: liq
POLY_3:
POLY_3: map
Version R mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point  1
Generating start point  2
Generating start point  3
Generating start point  4
Generating start point  5
Generating start point  6
Generating start point  7
Generating start point  8
Generating start point  9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14
Generating start point 15
Generating start point 16

Phase region boundary  1 at:    5.118E-02  2.000E-02  1.446E+03
** LIQUID
** CEMENTITE
FCC_A1
Terminating at diagram limit
CALCULATED          7 EQUILIBRIA

Phase region boundary  2 at:    5.118E-02  2.000E-02  1.446E+03
** LIQUID
** CEMENTITE
FCC_A1
CALCULATED          6 EQUILIBRIA

Phase region boundary  2 at:    8.299E-02  4.133E-02  1.467E+03
** LIQUID
** CEMENTITE
FCC_A1
M7C3

Phase region boundary  2 at:    3.000E-01  2.339E-01  1.467E+03
** LIQUID
** CEMENTITE
M7C3
Terminating at known equilibrium
CALCULATED          3 EQUILIBRIA

Phase region boundary  2 at:    8.299E-02  4.133E-02  1.467E+03
** LIQUID
FCC_A1
** M7C3
CALCULATED          24 EQUILIBRIA

Phase region boundary  2 at:    3.564E-02  2.106E-01  1.567E+03
** LIQUID
BCC_A2
FCC_A1
** M7C3

Phase region boundary  2 at:    3.000E-01  5.271E-01  1.567E+03
** LIQUID
** BCC_A2
M7C3
*** SORRY CANNOT CONTINUE *** 17

Phase region boundary  2 at:    3.564E-02  2.106E-01  1.567E+03

```

```

** LIQUID
** BCC_A2
FCC_A1
Terminating at diagram limit
CALCULATED 35 EQUILIBRIA
SKIPPING LINE WITHOUT LIQUID#1
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary 2 at: 2.557E-02 2.000E-02 1.446E+03
** LIQUID
** CEMENTITE
FCC_A1
Terminating at diagram limit
CALCULATED 7 EQUILIBRIA

Phase region boundary 2 at: 2.557E-02 2.000E-02 1.446E+03
** LIQUID
** CEMENTITE
FCC_A1
Terminating at known equilibrium
CALCULATED 6 EQUILIBRIA

Phase region boundary 2 at: 2.160E-01 2.000E-02 1.456E+03
LIQUID
** CEMENTITE
** GRAPHITE
Terminating at diagram limit
CALCULATED 9 EQUILIBRIA

Phase region boundary 2 at: 2.160E-01 2.000E-02 1.456E+03
LIQUID
** CEMENTITE
** GRAPHITE
CALCULATED 8 EQUILIBRIA

Phase region boundary 2 at: 2.034E-01 5.587E-02 1.500E+03
LIQUID
** CEMENTITE
** GRAPHITE
M7C3
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary 2 at: 2.034E-01 5.587E-02 1.500E+03
LIQUID
** CEMENTITE
** M7C3
Terminating at known equilibrium
CALCULATED 7 EQUILIBRIA

Phase region boundary 2 at: 2.034E-01 5.587E-02 1.500E+03
LIQUID
** GRAPHITE
** M7C3
CALCULATED 55 EQUILIBRIA

Phase region boundary 2 at: 3.484E-01 4.662E-01 1.863E+03
LIQUID
** GRAPHITE
M3C2
** M7C3
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary 2 at: 3.484E-01 4.662E-01 1.863E+03
LIQUID
** GRAPHITE
** M3C2
*** SORRY CANNOT CONTINUE *** 4

CALCULATED 33 EQUILIBRIA

Phase region boundary 2 at: 3.484E-01 4.662E-01 1.863E+03
LIQUID
** M3C2
** M7C3
*** SORRY CANNOT CONTINUE *** 4

CALCULATED 28 EQUILIBRIA

Phase region boundary 2 at: 2.249E-01 2.000E-02 1.456E+03
LIQUID
** CEMENTITE
** GRAPHITE
Terminating at diagram limit
CALCULATED 9 EQUILIBRIA

Phase region boundary 2 at: 2.249E-01 2.000E-02 1.456E+03
LIQUID
** CEMENTITE
** GRAPHITE
Terminating at known equilibrium
CALCULATED 8 EQUILIBRIA

Phase region boundary 2 at: 2.338E-01 2.000E-02 1.456E+03
LIQUID
** CEMENTITE
** GRAPHITE
Terminating at diagram limit
CALCULATED 9 EQUILIBRIA

Phase region boundary 2 at: 2.338E-01 2.000E-02 1.456E+03
LIQUID
** CEMENTITE
** GRAPHITE
Terminating at known equilibrium
CALCULATED 8 EQUILIBRIA

Phase region boundary 2 at: 2.428E-01 2.000E-02 1.456E+03
LIQUID
** CEMENTITE
** GRAPHITE
Terminating at diagram limit
CALCULATED 9 EQUILIBRIA

Phase region boundary 2 at: 2.428E-01 2.000E-02 1.456E+03
LIQUID
** CEMENTITE

```

```

** GRAPHITE
Terminating at known equilibrium
CALCULATED      8 EQUILIBRIA

Phase region boundary  2 at:   2.518E-01  2.000E-02  1.456E+03
LIQUID
** CEMENTITE
** GRAPHITE
Terminating at diagram limit
CALCULATED      9 EQUILIBRIA

Phase region boundary  2 at:   2.518E-01  2.000E-02  1.456E+03
LIQUID
** CEMENTITE
** GRAPHITE
Terminating at known equilibrium
CALCULATED      8 EQUILIBRIA

Phase region boundary  2 at:   3.427E-02  6.000E-01  1.660E+03
LIQUID
** BCC_A2
** M23C6
CALCULATED     21 EQUILIBRIA

Phase region boundary  2 at:   1.036E-01  4.168E-01  1.582E+03
LIQUID
** BCC_A2
** M23C6
M7C3
SKIPPING LINE WITHOUT LIQUID#1

Phase region boundary  2 at:   1.036E-01  4.168E-01  1.582E+03
LIQUID
** BCC_A2
** M7C3
Terminating at known equilibrium
CALCULATED     13 EQUILIBRIA

Phase region boundary  2 at:   1.036E-01  4.168E-01  1.582E+03
LIQUID
** M23C6
** M7C3
*** SORRY CANNOT CONTINUE ***    4

CALCULATED     47 EQUILIBRIA

Phase region boundary  2 at:   3.427E-02  6.000E-01  1.660E+03
LIQUID
** BCC_A2
** M23C6
*** SORRY CANNOT CONTINUE ***    4

*** LAST BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex46\fecr
c.POLY3
CPU time for mapping                2 seconds

```

```

POLY_3:
POLY_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

```

```

Setting automatic diagram axes

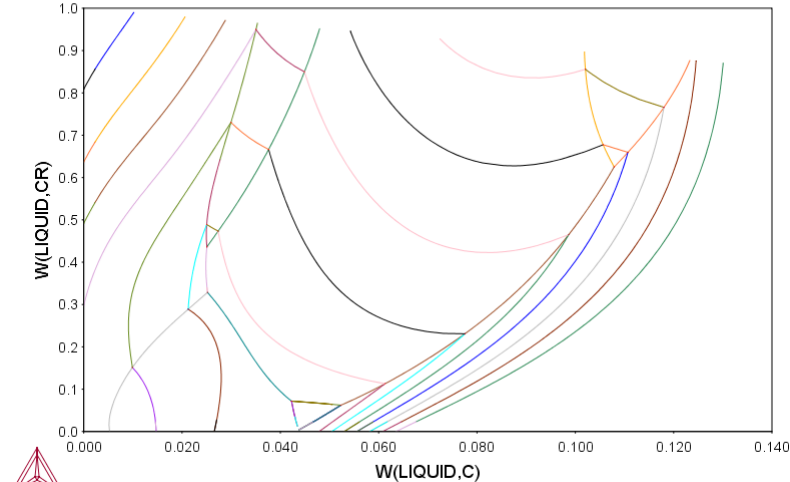
POST: s-d-a x W(liquid,c)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y W(liquid,cr)
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 46d
POST:
POST: plot
... the command in full is PLOT DIAGRAM

```

```

2016.05.16 14:42:56
TCFE7: C, CR, FE
N=1., P=1E5

```



```

POST:
POST:Hit RETURN to continue
POST: @@ Enter the table for the calculated data.
POST: e-sym tab tabl
... the command in full is ENTER_SYMBOL
Variable(s): W(liquid,c),W(liquid,cr),Temp_c;
POST:
POST: @@ Save the table on file
POST: tab tabl fecrc_liq.tab
... the command in full is TABULATE

```

```

POST:
POST: @@ Set the axis variables and the axis text for the final diagram
POST: s-a-t-s x n
... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Wei-Frac C
POST: s-a-t-s y n
... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Wei-Frac Cr
POST:
POST: s-d-a z temp-c
... the command in full is SET_DIAGRAM_AXIS
POST: s-a-t-s z n
... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Temp C
POST:
POST: @@ Specify the diagram type to be traingular
POST: s-d-t y,,,,
... the command in full is SET_DIAGRAM_TYPE
POST:
POST: @@ Finally, create the 3D-diagram (or .wrl file) by merging data
POST: @@ from the different tables created and saved. This is accomplished
POST: @@ using the command "CREATE_3D_DIAGRAM". Also define the scaling
POST: @@ to be used in the 3D-diagram.
POST: cre-3d
... the command in full is CREATE_3D_PLOTFILE
Use current WORKSPACE (WS), TAB files or BOTH: /WS/: BOTH
The table must contain values for X,Y and Z axis
DEFINED CONSTANTS
ZERO=0
DEFINED FUNCTIONS AND VARIABLES%
TEMP_C=T-273.15
DEFINED TABLES
TAB1=W(LIQUID,C), W(LIQUID,CR), TEMP_C
Table Name: tabl
Give TAB filename: /Cancel_to_finish/: fec_liq.tab fecr_liq.tab crc_liq.tab Cancel_to
Output file: /3Dplot/: tcex46_tri.wrl
X-AXIS SCALING FROM 0.0 TO XMAX /1/: 1
Y-AXIS SCALING FROM 0.0 TO YMAX /1/: 1
Z-AXIS SCALING, GIVE ZMIN /0/: 1200
Z-AXIS SCALING, GIVE ZMAX /2000/: 4600

It is possible to combine files by:
Copy Ter.tab+Bin1.tab+Bin2.tab+Bin3.tab Tmp.tab

Processing fec_liq.tab
3.4429100000000000E-009 <X< 1.0000000000000000
0.0000000000000000E+000 <Y< 0.0000000000000000E+000
1153.44000000000 <Z< 4500.07000000000

Processing fecr_liq.tab
0.0000000000000000E+000 <X< 0.0000000000000000E+000
1.1746300000000000E-009 <Y< 1.0000000000000000
1515.56000000000 <Z< 1919.76000000000

Processing crc_liq.tab
3.4411000000000000E-009 <X< 1.0000000000000000
3.3435800000000000E-008 <Y< 1.0000000000000000
1533.06000000000 <Z< 4492.14000000000
POST: ,,,,,,
No such command, use HELP
POST:
POST: @@ Change the diagram type to obtain a squared diagram
POST: s-d-t n,,,,
... the command in full is SET_DIAGRAM_TYPE
POST:
POST: @@ Create the squared 3D-diagram
POST: cre-3d
... the command in full is CREATE_3D_PLOTFILE
Use current WORKSPACE (WS), TAB files or BOTH: /WS/: BOTH
The table must contain values for X,Y and Z axis
DEFINED CONSTANTS
ZERO=0
DEFINED FUNCTIONS AND VARIABLES%
TEMP_C=T-273.15
DEFINED TABLES
TAB1=W(LIQUID,C), W(LIQUID,CR), TEMP_C
Table Name: tabl
Give TAB filename: /Cancel_to_finish/: fec_liq.tab fecr_liq.tab crc_liq.tab Cancel_to
Output file: /3Dplot/: tcex46_sqrt.wrl
X-AXIS SCALING FROM 0.0 TO XMAX /1/: .12
Y-AXIS SCALING FROM 0.0 TO YMAX /1/: 1
Z-AXIS SCALING, GIVE ZMIN /0/: 1200
Z-AXIS SCALING, GIVE ZMAX /2000/: 2200

It is possible to combine files by:
Copy Ter.tab+Bin1.tab+Bin2.tab+Bin3.tab Tmp.tab

Processing fec_liq.tab
3.4429100000000000E-009 <X< 1.0000000000000000
0.0000000000000000E+000 <Y< 0.0000000000000000E+000
1153.44000000000 <Z< 4500.07000000000

Processing fecr_liq.tab
0.0000000000000000E+000 <X< 0.0000000000000000E+000
1.1746300000000000E-009 <Y< 1.0000000000000000
1515.56000000000 <Z< 1919.76000000000

Processing crc_liq.tab
3.4411000000000000E-009 <X< 1.0000000000000000
3.3435800000000000E-008 <Y< 1.0000000000000000
1533.06000000000 <Z< 4492.14000000000
POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:

```



tcex47

About Stockholm, Sweden

Software (build 9533) running on WinNT 64-bit wordlength  
Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118  
License library version: 8.5.1.0017  
Linked: Mon May 16 09:31:44 2016

SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex47\tcex47.TCM"SYS: set-echo

SYS: @@  
SYS: @@ 3D-Diagram  
SYS: @@ A quarternary diagram with the gamma volume in the  
SYS: @@ Fe-Cr-Ni-C system at 1373K  
SYS: @@  
SYS: @@ This file calculated the gamma volume in fe-cr-ni-c system at 1100C  
SYS: @@ Please note that in order to view the generated file, tcex47.wrl,  
SYS: @@ it's necessary to install a WRML(Wirtual Reality Modelling  
SYS: @@ Language) viewer to web browser in use. WRML viwers can be  
SYS: @@ downloaded witout any cost from e.g. www.parallelgraphics.com  
SYS: @@ and www.sim.no

SYS:  
SYS: set-log ex47

Heading:

SYS: @@ Calculate the Fe-Cr-C side of the diagram  
SYS: go data

... the command in full is GOTO\_MODULE  
THERMODYNAMIC DATABASE module  
Current database: Steels/Fe-Alloys v8.0

VA DEFINED  
L12\_FCC B2\_BCC B2\_VACANCY  
HIGH\_SIGMA DICTRA\_FCC\_A1 REJECTED

TDB\_TCFE8: sw FEDEMO  
... the command in full is SWITCH\_DATABASE  
Current database: Iron Demo Database

VA /- DEFINED  
TDB\_FEDEMO: rej-sys

... the command in full is REJECT  
VA /- DEFINED

REINITIATING GES5 .....  
TDB\_FEDEMO: de-sys fe cr c  
... the command in full is DEFINE\_SYSTEM

FE CR C  
DEFINED

TDB\_FEDEMO: rej-ph \* all  
... the command in full is REJECT  
GAS:G LIQUID:L BCC\_A2  
CEMENTITE CHI\_A12 DIAMOND\_FCC\_A4  
FCC\_A1 GRAPHITE HCP\_A3  
KSI\_CARBIIDE LAVES\_PHASE\_C14 M23C6  
M3C2 M5C2 M7C3  
SIGMA REJECTED

TDB\_FEDEMO: res-ph fcc\_a1,bcc\_a2,m23,m7,ceMENTite  
... the command in full is RESTORE  
FCC\_A1 BCC\_A2 M23C6  
M7C3 CEMENTITE RESTORED

TDB\_FEDEMO: get  
... the command in full is GET\_DATA  
REINITIATING GES5 .....  
ELEMENTS .....  
SPECIES .....  
PHASES .....  
... the command in full is AMEND\_PHASE\_DESCRIPTION  
... the command in full is AMEND\_PHASE\_DESCRIPTION  
PARAMETERS ...  
FUNCTIONS ....

List of references for assessed data

'J-O. Andersson, Calphad, 11 (1987), 271-276; TRITA 0314; C-CR'  
'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'  
'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo -C, C-Mn'  
'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C  
-FE'  
'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'  
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;  
Molar volumes'  
'X.-G. Lu et al. Calphad 29 (2005) 49-55, Fe P-T diagram'  
'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'  
'J-O. Andersson, Metall. Trans. A, 19A (1988), 627-636 TRITA 0207 (1986);  
C-CR-FE'  
'J-O. Andersson and B. Sundman, Calphad, 11 (1987), 83-92; TRITA 0270  
(1986); CR-FE'  
'P. Villars and L.D. Calvert (1985). Pearsons handbook of crystallographic  
data for intermetallic phases. Metals park, Ohio. American Society for  
Metals; Molar volumes'  
'J. Bratberg, Z. Metallkd., Vol 96 (2005), 335-344; Fe-Cr-Mo-C'  
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'  
-OK-

TDB\_FEDEMO:

TDB\_FEDEMO: go poly  
... the command in full is GOTO\_MODULE

POLY version 3.32  
POLY\_3: s-c t=1373  
... the command in full is SET\_CONDITION  
POLY\_3: se-co n=1,p=1e5  
... the command in full is SET\_CONDITION  
POLY\_3: se-co x(c)=.01  
... the command in full is SET\_CONDITION  
POLY\_3: se-co x(cr)=.05  
... the command in full is SET\_CONDITION  
POLY\_3: c-e  
... the command in full is COMPUTE\_EQUILIBRIUM  
Using global minimization procedure  
Calculated 5731 grid points in 0 s  
Found the set of lowest grid points in 0 s  
Calculated POLY solution 0 s, total time 0 s  
POLY\_3:  
POLY\_3: s-a-v 1 x(c) 0 1 .01

```

... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(cr) 0 1 .01
... the command in full is SET_AXIS_VARIABLE
POLY_3: add-in 1,,,,,
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: advanced
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /NONE/: fcc_a1
POLY_3: save tcex47 y
... the command in full is SAVE_WORKSPACES
POLY_3: map
Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2

Phase region boundary 1 at: 1.765E-01 1.880E-01
FCC_A1
** M7C3
Calculated. 5 equilibria

Phase region boundary 2 at: 1.830E-01 1.507E-01
** CEMENTITE
FCC_A1
** M7C3

Phase region boundary 3 at: 1.580E-01 9.227E-02
** CEMENTITE
FCC_A1
Calculated 25 equilibria

Phase region boundary 4 at: 1.830E-01 1.507E-01
FCC_A1
** M7C3
Calculated. 23 equilibria

Phase region boundary 5 at: 1.589E-01 3.687E-01
FCC_A1
** M23C6
** M7C3

Phase region boundary 6 at: 1.123E-01 3.478E-01
FCC_A1
** M23C6
Calculated. 2 equilibria

Phase region boundary 7 at: 1.122E-01 3.494E-01
** BCC_A2
FCC_A1
** M23C6

Phase region boundary 8 at: 1.066E-02 1.975E-01
** BCC_A2
FCC_A1
Calculated 23 equilibria

Phase region boundary 9 at: 1.765E-01 1.880E-01
FCC_A1
** M7C3
Calculated. 20 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex47\tcex
47.POLY3
CPU time for mapping 0 seconds
POLY_3:
POLY_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

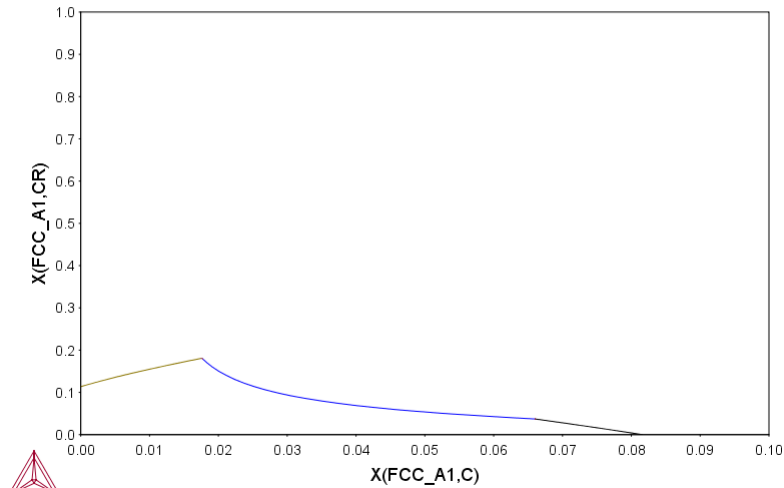
Setting automatic diagram axes

POST: s-d-a x x(fcc_a1,c)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y x(fcc_a1,cr)
... the command in full is SET_DIAGRAM_AXIS
POST: s-s-s x n 0 .1
... the command in full is SET_SCALING_STATUS
POST: s-s-s y n 0 1
... the command in full is SET_SCALING_STATUS
POST: set-title example 47a
POST: plot
... the command in full is PLOT_DIAGRAM

```

# example 47a

2016.05.16.14.44.36  
FEDEMO: C, CR, FE  
T=1373, N=1, P=1E5



```
POST:
POST:Hit RETURN to continue
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the Cr content in the fcc_a1 phase, in the second Ni content which is "zero"
POST: @@ here, and in the last column the C content of the fcc_a1 phase.
POST: e-sym tab tab1
... the command in full is ENTER_SYMBOL
Variable(s): x(fcc_a1,cr),ZERO,x(fcc_a1,c)
&
POST: @@ Save the tabulated data on file
POST: tab tab1 fecrc_1373.tab
... the command in full is TABULATE
POST: back
POLY_3:
POLY_3: @@ Calculate the Fe-Cr-ni side of the diagram
POLY_3: go data
... the command in full is GOTO_MODULE
TDB_FEDEMO: rej-sys
... the command in full is REJECT
VA
REINITIATING GES5 .....
TDB_FEDEMO: de-sys fe cr ni
... the command in full is DEFINE_SYSTEM
FE          CR          NI
DEFINED
TDB_FEDEMO: rej-ph * all
... the command in full is REJECT
LIQUID:L          BCC_A2          CHI_A12
FCC_A1          HCP_A3          LAVES_PHASE_C14
SIGMA REJECTED
TDB_FEDEMO: res-ph bcc_a2, fcc_a1
... the command in full is RESTORE
BCC_A2          FCC_A1 RESTORED
TDB_FEDEMO: get
... the command in full is GET_DATA
REINITIATING GES5 .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....
```

List of references for assessed data

'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'  
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;  
Molar volumes'  
'X.-G. Lu et al. Calphad 29 (2005) 49-55, Fe P-T diagram'  
'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'  
'J.-O. Andersson and B. Sundman, Calphad, 11 (1987), 83-92; TRITA 0270  
(1986); CR-FE'  
'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'  
'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR-NI'  
'A. Dinsdale, T. Chart, MTDS NPL, unpublished work (1986); FE-NI'  
-OK-

```
TDB_FEDEMO:
TDB_FEDEMO: go poly
... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3: s-c t=1373
... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
... the command in full is SET_CONDITION
POLY_3: se-co x(ni)=.005
... the command in full is SET_CONDITION
POLY_3: se-co x(cr)=.005
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 3954 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY_3:
POLY_3: s-a-v 1 x(ni) 0 1 .01
... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(cr) 0 1 .01
... the command in full is SET_AXIS_VARIABLE
```

```

POLY_3: add-in 2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add-in 1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: advanced
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /NONE/: fcc_a1
POLY_3: save tcex47 y
... the command in full is SAVE_WORKSPACES

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

POLY_3: map
Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Working hard
Generating start point 1
Generating start point 2

Phase region boundary 1 at: 4.206E-03 1.318E-01
** BCC_A2
FCC_A1
Calculated 12 equilibria

Phase region boundary 2 at: 4.206E-03 1.318E-01
** BCC_A2
FCC_A1
Calculated 86 equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex47\tcex
47.POLY3
CPU time for mapping 1 seconds

```

```

POLY_3:
POLY_3: post

```

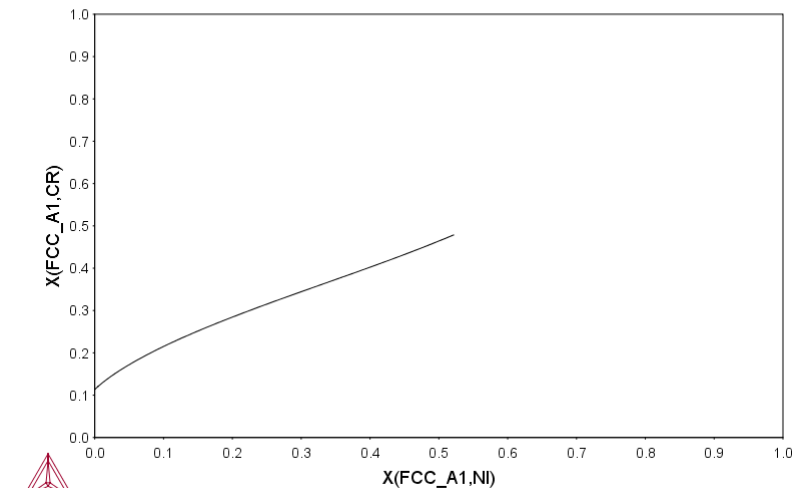
```

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST: s-d-a x x(fcc_a1,ni)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y x(fcc_a1,cr)
... the command in full is SET_DIAGRAM_AXIS
POST: s-s-s x n 0 1
... the command in full is SET_SCALING_STATUS
POST: s-s-s y n 0 1
... the command in full is SET_SCALING_STATUS
POST: set-title example 47b
POST:
POST: plot
... the command in full is PLOT DIAGRAM

```



```

POST:
POST:
POST:Hit RETURN to continue
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the Cr content in the fcc_a1 phase, in the second Ni content
POST: @@ and in the last column the C content of the fcc_a1 phase, which is zero
POST: e-sym tab tab2
... the command in full is ENTER_SYMBOL
Variable(s): x(fcc_a1,cr),x(fcc_a1,ni),zero
&
POST: @@ Save the tabulated data on file
POST: tab tab2 fecrni_1373.tab
... the command in full is TABULATE
POST: back
POLY_3:
POLY_3: @@ Calculate the Fe-C-Ni side of the diagram
POLY_3: go data
... the command in full is GOTO_MODULE
TDB_FEDEMO: rej-sys
... the command in full is REJECT
VA /- DEFINED
REINITIATING GES5 .....

```

```

TDB_FEDEMO: de-sys fe Ni C
... the command in full is DEFINE_SYSTEM
FE          NI          C
DEFINED
TDB_FEDEMO: rej-ph * all
... the command in full is REJECT
GAS:G          LIQUID:L          BCC_A2
CEMENTITE          DIAMOND_FCC_A4          FCC_A1
GRAPHITE          HCP_A3          KSI_CARBIDE
LAVES_PHASE_C14          M23C6          M5C2
M7C3 REJECTED
TDB_FEDEMO: res-ph fcc_a1,bcc_a2,cementite,hcp_a3
... the command in full is RESTORE
FCC_A1          BCC_A2          CEMENTITE
HCP_A3 RESTORED
TDB_FEDEMO: get
... the command in full is GET_DATA
REINITIATING GES5 .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo -C, C-Mn'
'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
-FE'
'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
'A. Gabriel, C. Chatillon, and I. Ansara, published in High Temp. Sci.
(parameters listed in Calphad, 11 (1987), 203-218); C-NI'
'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
Molar volumes'
'X.-G. Lu et al. Calphad 29 (2005) 49-55, Fe P-T diagram'
'A. Gabriel, P. Gustafson, and I. Ansara, Calphad, 11 (1987), 203 -218;
TRITA-MAC 285 (1986); C-FE-NI'
'A. Dinsdale, T. Chart, MTDS NPL, unpublished work (1986); FE-NI'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'
'A. Fernandez Guillermet, Z. Metallkde., 79 (1988), 524-536, TRITA -MAC
362 (1988); C-CO-NI AND C-CO-FE-NI'
-OK-
TDB_FEDEMO:
TDB_FEDEMO: go poly
... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3: s-c t=1373
... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
... the command in full is SET_CONDITION
POLY_3: se-co x(C)=.005
... the command in full is SET_CONDITION
POLY_3: se-co x(ni)=.005
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated          5594 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution          0 s, total time          0 s
POLY_3:
POLY_3: s-a-v 1 x(c) 0 1 .01
... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(ni) 0 1 .01
... the command in full is SET_AXIS_VARIABLE
POLY_3: add-in 2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add-in 1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: advanced
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /NONE/: fcc_a1
POLY_3:
POLY_3: save tcex47 y
... the command in full is SAVE_WORKSPACES

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

POLY_3: map
Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Generating start point 1
Generating start point 2

Phase region boundary 1 at: 1.657E-01 3.147E-03
** CEMENTITE
FCC_A1
Calculated          9 equilibria

Phase region boundary 2 at: 1.657E-01 3.147E-03
** CEMENTITE
FCC_A1
Calculated          104 equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex47\tcex
47.POLY3
CPU time for mapping          0 seconds
POLY_3:
POLY_3: post

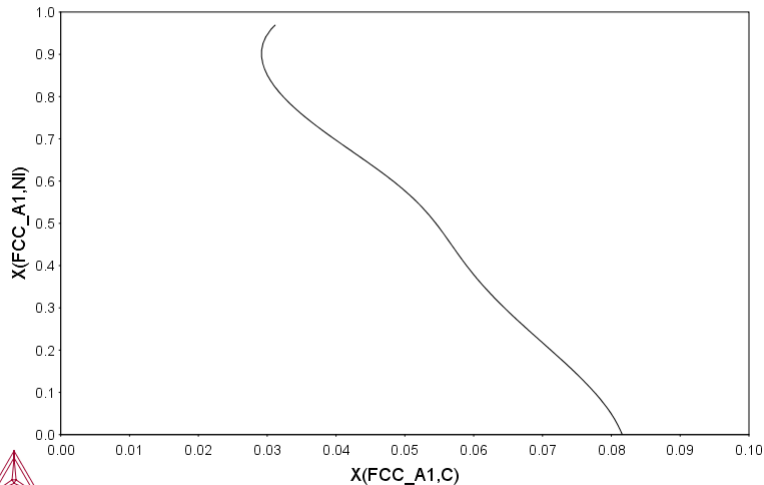
```

Setting automatic diagram axes

```
POST: s-d-a x x(fcc_a1,c)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y x(fcc_a1,ni)
... the command in full is SET_DIAGRAM_AXIS
POST: s-s-s x n 0 .1
... the command in full is SET_SCALING_STATUS
POST: s-s-s y n 0 1
... the command in full is SET_SCALING_STATUS
POST: set-title example 47c
POST:
POST: plot
... the command in full is PLOT DIAGRAM
```

example 47c

2016.05.16.14.44.41  
FEDEMO: C, FE, NI  
T=1373, N=1, P=1E5



```
POST:
POST:Hit RETURN to continue
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the Cr content in the fcc_a1 phase, in the second Ni
POST: @@ and in the last column the C content of the fcc_a1 phase.
POST: e-sym tab tab3
... the command in full is ENTER_SYMBOL
Variable(s): zero,x(fcc_a1,ni),x(fcc_a1,c)
&
POST: @@ Save the tabulated data on file
POST: tab tab3 fenic_1373.tab
... the command in full is TABULATE
POST: back
POLY_3:
POLY_3: @@ Calculate the Cr-ni-C side of the diagram
POLY_3: go data
... the command in full is GOTO_MODULE
TDB_FEDEMO: rej-sys
... the command in full is REJECT
VA /- DEFINED
REINITIATING GES5 .....
TDB_FEDEMO: de-sys cr ni C
... the command in full is DEFINE_SYSTEM
CR NI C
DEFINED
TDB_FEDEMO:
TDB_FEDEMO: rej-ph * all
... the command in full is REJECT
GAS:G LIQUID:L BCC_A2
CEMENTITE CHI_A12 DIAMOND_FCC_A4
FCC_A1 GRAPHITE HCP_A3
KSI_CARBIDE LAVES_PHASE_C14 M23C6
M3C2 M7C3 SIGMA
REJECTED
TDB_FEDEMO: res-ph fcc_a1,bcc_a2,ceementite,hcp_a3
... the command in full is RESTORE
FCC_A1 BCC_A2 CEMENTITE
HCP_A3 RESTORED
TDB_FEDEMO: get
... the command in full is GET_DATA
REINITIATING GES5 .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....
```

List of references for assessed data

'J-O. Andersson, Calphad, 11 (1987), 271-276; TRITA 0314; C-CR'  
'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'  
'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo -C, C-Mn'  
'A. Gabriel, C. Chatillon, and I. Ansara, published in High Temp. Sci.  
(parameters listed in Calphad, 11 (1987), 203-218); C-NI'  
'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'  
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;  
Molar volumes'  
'NPL, unpublished work (1989); C-Cr-Ni'  
'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'  
'A. Dinsdale and T. Chart, MTDS NPL, Unpublished work (1986); CR-NI'  
'P. Villars and L.D. Calvert (1985). Pearsons handbook of crystallographic

```

data for intermetallic phases. Metals park, Ohio. American Society for
Metals; Molar volumes'
'A. Gabriel, P. Gustafson, and I. Ansara, Calphad, 11 (1987), 203 -218;
TRITA-MAC 285 (1986); C-FE-NI'
'A. Markstrom, Swerea KIMAB, Sweden; Molar volumes'
'J. Bratberg, Z. Metallkd., Vol 96 (2005), 335-344; Fe-Cr-Mo-C'
'C. Qiu, ISIJ International, 32 (1992), 1117-1127; C-Cr-Fe-Mo'
'A. Fernandez Guillermet, Z. Metallkde., 79 (1988), 524-536, TRITA -MAC
362 (1988); C-CO-NI AND C-CO-FE-NI'
'P. Gustafson, Metall. Trans. A, 19A (1988), 2547-2554; TRITA-MAC 348,
(1987); C-CR-FE-W'

```

-OK-

**TDB\_FEDEMO:**

**TDB\_FEDEMO:** go poly

... the command in full is GOTO\_MODULE

POLY version 3.32

**POLY\_3:** s-c t=1373

... the command in full is SET\_CONDITION

**POLY\_3:** se-co n=1,p=1e5

... the command in full is SET\_CONDITION

**POLY\_3:** se-co x(C)=.005

... the command in full is SET\_CONDITION

**POLY\_3:** se-co x(cr)=.005

... the command in full is SET\_CONDITION

**POLY\_3:** c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Using global minimization procedure

```

Calculated          5594 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution          0 s, total time  0 s

```

**POLY\_3:**

**POLY\_3:** s-a-v 1 x(c) 0 1 .01

... the command in full is SET\_AXIS\_VARIABLE

**POLY\_3:** s-a-v 2 x(cr) 0 1 .01

... the command in full is SET\_AXIS\_VARIABLE

**POLY\_3:** add-in 2

... the command in full is ADD\_INITIAL\_EQUILIBRIUM

**POLY\_3:** add-in 1

... the command in full is ADD\_INITIAL\_EQUILIBRIUM

**POLY\_3:**

**POLY\_3:** advanced

... the command in full is ADVANCED\_OPTIONS

**Which option? /STEP\_AND\_MAP/:** present

**Phase name /NONE/:** fcc\_a1

**POLY\_3:**

**POLY\_3:** save tcex47 y

... the command in full is SAVE\_WORKSPACES

This file contains results from a previous STEP or MAP command.

The SAVE command will save the current status of the program but destroy the results from the previous STEP or MAP commands.

**POLY\_3:** map

Version S mapping is selected

Organizing start points

Using ADDED start equilibria

```

Generating start point  1
Generating start point  2

```

Phase region boundary 1 at: 1.410E-01 4.254E-03

\*\* CEMENTITE

FCC\_A1

Calculated 10 equilibria

Phase region boundary 2 at: 1.410E-01 4.254E-03

\*\* CEMENTITE

FCC\_A1

Calculated. 14 equilibria

Phase region boundary 3 at: 1.475E-01 1.250E-01

\*\* CEMENTITE

FCC\_A1

\*\* FCC\_A1#2

Phase region boundary 4 at: 2.681E-01 3.002E-01

FCC\_A1

\*\* FCC\_A1#2

Calculated. 7 equilibria

Calculated 7 equilibria

Phase region boundary 5 at: 2.681E-01 3.002E-01

FCC\_A1

\*\* FCC\_A1#2

Calculated. 4 equilibria

Phase region boundary 6 at: 2.545E-01 3.227E-01

FCC\_A1

\*\* FCC\_A1#2

\*\* HCP\_A3

Phase region boundary 7 at: 1.819E-01 3.945E-01

FCC\_A1

\*\* HCP\_A3

Calculated. 14 equilibria

Phase region boundary 8 at: 1.520E-01 5.236E-01

\*\* CEMENTITE

FCC\_A1

\*\* HCP\_A3

Phase region boundary 9 at: 1.267E-01 5.426E-01

\*\* CEMENTITE

FCC\_A1

Calculated. 8 equilibria

Phase region boundary 10 at: 1.262E-01 6.075E-01

\*\* BCC\_A2

\*\* CEMENTITE

FCC\_A1

Phase region boundary 11 at: 1.249E-03 6.835E-01

```

** BCC_A2
   FCC_A1
Calculated                      13 equilibria

Phase region boundary 12 at:   1.475E-01  1.250E-01
** CEMENTITE
   FCC_A1
Calculated                      27 equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex47\tcex
47.POLY3
CPU time for mapping              0 seconds
POLY_3:
POLY_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

```

Setting automatic diagram axes

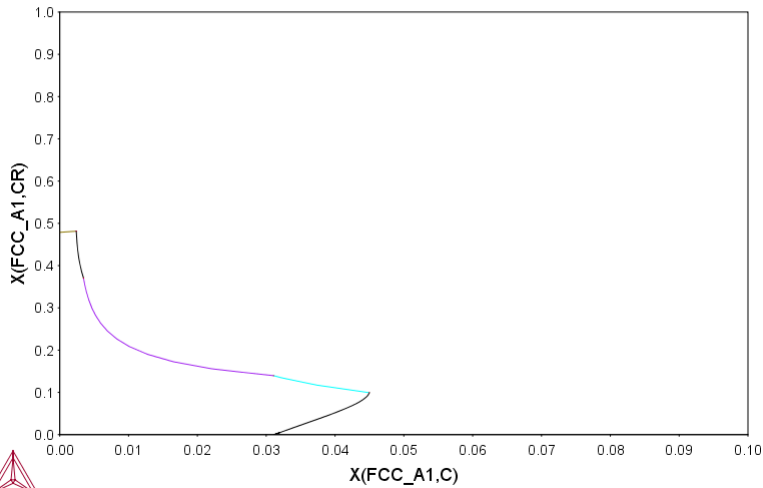
```

POST: s-d-a x x(fcc_a1,c)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y x(fcc_a1,cr)
... the command in full is SET_DIAGRAM_AXIS
POST: s-s-s x n 0 .1
... the command in full is SET_SCALING_STATUS
POST: s-s-s y n 0 1
... the command in full is SET_SCALING_STATUS
POST: set-title example 47d
POST:
POST: plot
... the command in full is PLOT DIAGRAM

```

**example 47d**

2016.05.16.14.44.43  
FEDEMO: C, CR, NI  
T=1373, N=1, P=1E5



```

POST:
POST: Hit RETURN to continue
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the Cr content in the fcc_a1 phase, in the second Ni content
POST: @@ and in the last column the C content of the fcc_a1 phase.
POST: e-sym tab tab4
... the command in full is ENTER_SYMBOL
Variable(s): x(fcc_a1,cr),x(fcc_a1,ni),x(fcc_a1,c)
&
POST: @@ Save the tabulated data on file
POST: tab tab4 crnic_1373.tab
... the command in full is TABULATE
POST: back
POLY_3:
POLY_3:
POLY_3: @@ Next calculate a projection of the Fe-Cr-ni-C system
POLY_3: go data
... the command in full is GOTO_MODULE
TDB_FEDEMO: rej-sys
... the command in full is REJECT
VA /- DEFINED
REINITIATING GES5 .....
TDB_FEDEMO: de-sys fe cr ni C
... the command in full is DEFINE_SYSTEM
FE CR NI
C DEFINED
TDB_FEDEMO: rej-ph * all
... the command in full is REJECT
GAS:G LIQUID:L BCC_A2
CEMENTITE CHI_A12 DIAMOND_FCC_A4
FCC_A1 GRAPHITE HCP_A3
KSI_CARBIDE LAVES_PHASE_C14 M23C6
M3C2 M5C2 M7C3
SIGMA REJECTED
TDB_FEDEMO: res-ph fcc_a1,bcc_a2,hcp_a3,m23,fcc_a1,bcc_a2,m23,m7, cementite
... the command in full is RESTORE
FCC_A1 BCC_A2 HCP_A3
M23C6 M7C3 CEMENTITE
RESTORED
TDB_FEDEMO: get
... the command in full is GET_DATA
REINITIATING GES5 .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...

```



FUNCTIONS ....

List of references for assessed data

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-OK-

**TDB\_FEDEMO:**

**TDB\_FEDEMO:** go poly

... the command in full is GOTO\_MODULE

POLY version 3.32

**POLY\_3:** s-c t=1373

... the command in full is SET\_CONDITION

**POLY\_3:** se-co n=1,p=1e5

... the command in full is SET\_CONDITION

**POLY\_3:** se-co x(C)=.05

... the command in full is SET\_CONDITION

**POLY\_3:** se-co x(ni)=.005

... the command in full is SET\_CONDITION

**POLY\_3:** se-co x(fcc\_al,cr)=.02

... the command in full is SET\_CONDITION

**POLY\_3:**

**POLY\_3:** c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Normal POLY minimization, not global

Testing POLY result by global minimization procedure

Calculated 9750 grid points in 0 s  
33 ITS, CPU TIME USED 0 SECONDS

**POLY\_3:**

**POLY\_3:** s-a-v 1 x(c) 0 1 .005

... the command in full is SET\_AXIS\_VARIABLE

**POLY\_3:** s-a-v 2 x(ni) 0 1 .005

... the command in full is SET\_AXIS\_VARIABLE

**POLY\_3:** add-in 2

... the command in full is ADD\_INITIAL\_EQUILIBRIUM

**POLY\_3:** add-in 1

... the command in full is ADD\_INITIAL\_EQUILIBRIUM

**POLY\_3:**

**POLY\_3:** se-co x(C)=.05

... the command in full is SET\_CONDITION

**POLY\_3:** se-co x(ni)=.005

... the command in full is SET\_CONDITION

**POLY\_3:** se-co x(fcc\_al,cr)=.04

... the command in full is SET\_CONDITION

**POLY\_3:** c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Normal POLY minimization, not global

Testing POLY result by global minimization procedure

Using already calculated grid

15 ITS, CPU TIME USED 0 SECONDS

**POLY\_3:**

**POLY\_3:** add-in 2

... the command in full is ADD\_INITIAL\_EQUILIBRIUM

**POLY\_3:** add-in 1

... the command in full is ADD\_INITIAL\_EQUILIBRIUM

**POLY\_3:**

**POLY\_3:** se-co x(C)=.05

... the command in full is SET\_CONDITION

**POLY\_3:** se-co x(ni)=.005

... the command in full is SET\_CONDITION

**POLY\_3:** se-co x(fcc\_al,cr)=.06

... the command in full is SET\_CONDITION

**POLY\_3:** c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Normal POLY minimization, not global

Testing POLY result by global minimization procedure

Using already calculated grid

22 ITS, CPU TIME USED 0 SECONDS

**POLY\_3:**

**POLY\_3:** add-in 2

... the command in full is ADD\_INITIAL\_EQUILIBRIUM

**POLY\_3:** add-in 1

... the command in full is ADD\_INITIAL\_EQUILIBRIUM

**POLY\_3:**

**POLY\_3:** se-co x(C)=.05

... the command in full is SET\_CONDITION

**POLY\_3:** se-co x(ni)=.005

... the command in full is SET\_CONDITION

**POLY\_3:** se-co x(fcc\_al,cr)=.08

... the command in full is SET\_CONDITION

```

POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Using already calculated grid
17 ITS, CPU TIME USED 0 SECONDS
POLY_3:
POLY_3: add-in 2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add-in 1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-co x(C)=.05
... the command in full is SET_CONDITION
POLY_3: se-co x(ni)=.005
... the command in full is SET_CONDITION
POLY_3: se-co x(fcc_a1,cr)=.1
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Using already calculated grid
17 ITS, CPU TIME USED 0 SECONDS
POLY_3:
POLY_3: add-in 2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add-in 1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-co x(C)=.05
... the command in full is SET_CONDITION
POLY_3: se-co x(ni)=.005
... the command in full is SET_CONDITION
POLY_3: se-co x(fcc_a1,cr)=.12
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Using already calculated grid
17 ITS, CPU TIME USED 0 SECONDS
POLY_3:
POLY_3: add-in 2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add-in 1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: se-co x(C)=.05
... the command in full is SET_CONDITION
POLY_3: se-co x(ni)=.005
... the command in full is SET_CONDITION
POLY_3: se-co x(fcc_a1,cr)=.14
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Normal POLY minimization, not global
Testing POLY result by global minimization procedure
Using already calculated grid
18 ITS, CPU TIME USED 0 SECONDS
POLY_3:
POLY_3: add-in 2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add-in 1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-co x(C)=.05
... the command in full is SET_CONDITION
POLY_3: se-co x(ni)=.005
... the command in full is SET_CONDITION
POLY_3: se-co x(fcc_a1,cr)=.16c-e
... the command in full is SET_CONDITION
POLY_3:
POLY_3: add-in 2
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add-in 1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: advanced
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /NONE/: fcc_a1
POLY_3: save tcex47 y
... the command in full is SAVE_WORKSPACES

```

This file contains results from a previous STEP or MAP command.  
The SAVE command will save the current status of the program but destroy  
the results from the previous STEP or MAP commands.

```

POLY_3: map
Version S mapping is selected

```

Organizing start points

Using ADDED start equilibria

```

Tie-lines not in the plane of calculation
Generating start point 1
Generating start point 2
ERROR 1611 when calculating equilibrium
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
ERROR 1611 when calculating equilibrium
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Working hard
Generating start point 11
Generating start point 12
Generating start point 13
Generating start point 14

```

```

Generating start point 15
Generating start point 16
Generating start point 17
Generating start point 18
Generating start point 19
Generating start point 20
Working hard

Phase region boundary 1 at: 5.000E-02 2.951E-01
  FCC_A1
  ** M7C3
Calculated. 60 equilibria

Phase region boundary 2 at: 4.791E-02 5.888E-01
  ** CEMENTITE
  FCC_A1
  ** M7C3

Phase region boundary 3 at: 4.791E-02 5.888E-01
  CEMENTITE
  FCC_A1
  ** M7C3
Calculated. 38 equilibria
Terminating at known equilibrium

Phase region boundary 4 at: 4.791E-02 5.888E-01
  ** CEMENTITE
  FCC_A1
Calculated. 86 equilibria

Phase region boundary 5 at: 4.791E-02 5.888E-01
  ** CEMENTITE
  FCC_A1
  M7C3
Calculated. 87 equilibria
Terminating at known equilibrium

Phase region boundary 6 at: 4.791E-02 5.888E-01
  FCC_A1
  ** M7C3
Calculated. 75 equilibria

Phase region boundary 7 at: 5.851E-02 2.219E-01
  ** CEMENTITE
  FCC_A1
  ** M7C3

Phase region boundary 8 at: 5.851E-02 2.219E-01
  CEMENTITE
  FCC_A1
  ** M7C3
Calculated. 69 equilibria
Terminating at known equilibrium

Phase region boundary 9 at: 5.851E-02 2.219E-01
  ** CEMENTITE
  FCC_A1
Calculated. 60 equilibria

Phase region boundary 10 at: 5.851E-02 2.219E-01
  ** CEMENTITE
  FCC_A1
  M7C3
Calculated. 79 equilibria
Terminating at known equilibrium

Phase region boundary 11 at: 5.000E-02 2.951E-01
  FCC_A1
  ** M7C3
Calculated. 16 equilibria
Terminating at known equilibrium

Phase region boundary 12 at: 7.320E-02 5.000E-03
  ** CEMENTITE
  FCC_A1
Calculated. 22 equilibria

Phase region boundary 13 at: 7.320E-02 5.000E-03
  ** CEMENTITE
  FCC_A1
Calculated. 45 equilibria
Terminating at known equilibrium

Phase region boundary 14 at: 5.000E-02 8.665E-02
  FCC_A1
  ** M7C3
Calculated. 117 equilibria

Phase region boundary 15 at: 3.277E-02 6.655E-01
  FCC_A1
  ** FCC_A1#2
  ** M7C3

Phase region boundary 16 at: 3.277E-02 6.655E-01
  FCC_A1
  FCC_A1#2
  ** M7C3
Calculated. 134 equilibria
Terminating at known equilibrium

Phase region boundary 17 at: 3.277E-02 6.655E-01
  FCC_A1
  ** FCC_A1#2
Calculated. 15 equilibria

Phase region boundary 18 at: 3.930E-02 7.344E-01
  ** CEMENTITE
  FCC_A1
  ** FCC_A1#2

Phase region boundary 19 at: 3.930E-02 7.344E-01
  CEMENTITE
  FCC_A1
  ** FCC_A1#2
Calculated. 64 equilibria
Terminating at known equilibrium

```

Phase region boundary 20 at: 3.930E-02 7.344E-01  
 \*\* CEMENTITE  
 FCC\_A1  
 Calculated 49 equilibria

Phase region boundary 21 at: 3.930E-02 7.344E-01  
 \*\* CEMENTITE  
 FCC\_A1  
 FCC\_A1#2  
 Calculated. 147 equilibria  
 Terminating at known equilibrium

Phase region boundary 22 at: 3.277E-02 6.655E-01  
 FCC\_A1  
 \*\* FCC\_A1#2  
 M7C3  
 Calculated. 108 equilibria  
 Terminating at known equilibrium

Phase region boundary 23 at: 3.277E-02 6.655E-01  
 FCC\_A1  
 \*\* M7C3  
 Calculated 145 equilibria

Phase region boundary 24 at: 5.000E-02 8.665E-02  
 FCC\_A1  
 \*\* M7C3  
 Calculated 32 equilibria

Phase region boundary 25 at: 6.207E-02 5.000E-03  
 FCC\_A1  
 \*\* M7C3  
 Calculated 5 equilibria

Phase region boundary 26 at: 6.207E-02 5.000E-03  
 FCC\_A1  
 \*\* M7C3  
 Calculated. 134 equilibria  
 Terminating at known equilibrium

Phase region boundary 27 at: 3.000E-01 5.000E-03  
 \*\* FCC\_A1  
 M7C3  
 Calculated 10 equilibria

Phase region boundary 28 at: 3.000E-01 5.000E-03  
 \*\* FCC\_A1  
 M7C3  
 Calculated. 44 equilibria

Phase region boundary 29 at: 3.000E-01 1.229E-01  
 \*\* FCC\_A1  
 \*\* FCC\_A1#2  
 M7C3

Phase region boundary 30 at: 3.000E-01 1.229E-01  
 \*\* FCC\_A1  
 FCC\_A1#2  
 M7C3  
 Calculated. 48 equilibria  
 Terminating at known equilibrium

Phase region boundary 31 at: 3.000E-01 1.229E-01  
 FCC\_A1  
 \*\* FCC\_A1#2  
 M7C3  
 Calculated. 121 equilibria  
 Terminating at known equilibrium

Phase region boundary 32 at: 3.000E-01 1.229E-01  
 \*\* FCC\_A1  
 M7C3  
 Calculated 65 equilibria

Phase region boundary 33 at: 3.000E-01 5.000E-03  
 \*\* FCC\_A1  
 M7C3  
 Calculated 11 equilibria

Phase region boundary 34 at: 3.000E-01 5.000E-03  
 \*\* FCC\_A1  
 M7C3  
 Calculated. 45 equilibria

Phase region boundary 35 at: 3.000E-01 1.251E-01  
 \*\* FCC\_A1  
 \*\* FCC\_A1#2  
 M7C3

Phase region boundary 36 at: 3.000E-01 1.251E-01  
 \*\* FCC\_A1  
 FCC\_A1#2  
 M7C3  
 Calculated. 49 equilibria  
 Terminating at known equilibrium

Phase region boundary 37 at: 3.000E-01 1.251E-01  
 FCC\_A1  
 \*\* FCC\_A1#2  
 M7C3  
 Calculated. 131 equilibria  
 Terminating at known equilibrium

Phase region boundary 38 at: 3.000E-01 1.251E-01  
 \*\* FCC\_A1  
 M7C3  
 Calculated 63 equilibria

Phase region boundary 39 at: 3.000E-01 5.000E-03  
 \*\* FCC\_A1  
 M7C3  
 Calculated 11 equilibria

Phase region boundary 40 at: 3.000E-01 5.000E-03  
 \*\* FCC\_A1

```

M7C3
Calculated.                46 equilibria

Phase region boundary 41 at: 3.000E-01 1.310E-01
** FCC_A1
** FCC_A1#2
M7C3

Phase region boundary 42 at: 3.000E-01 1.310E-01
** FCC_A1
FCC_A1#2
M7C3
Calculated.                51 equilibria
Terminating at known equilibrium

Phase region boundary 43 at: 3.000E-01 1.310E-01
FCC_A1
** FCC_A1#2
M7C3
Calculated.                138 equilibria
Terminating at known equilibrium

Phase region boundary 44 at: 3.000E-01 1.310E-01
** FCC_A1
M7C3
Calculated                62 equilibria

Phase region boundary 45 at: 3.000E-01 5.000E-03
** FCC_A1
M7C3
Calculated                33 equilibria

Phase region boundary 46 at: 3.000E-01 5.000E-03
** FCC_A1
M7C3
Calculated                63 equilibria

Phase region boundary 47 at: 3.000E-01 5.000E-03
** FCC_A1
M7C3
Calculated                19 equilibria

Phase region boundary 48 at: 3.000E-01 5.000E-03
** FCC_A1
M7C3
Calculated                50 equilibria

Phase region boundary 49 at: 3.000E-01 5.000E-03
** FCC_A1
M7C3
Calculated                19 equilibria

Phase region boundary 50 at: 3.000E-01 5.000E-03
** FCC_A1
M7C3
Calculated                51 equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex47\tcex
47.POLY3
CPU time for mapping                10 seconds
POLY_3:
POLY_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

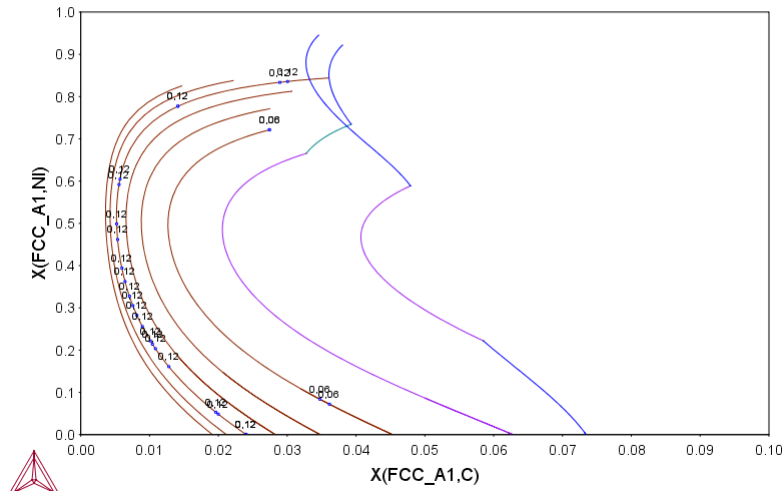
Setting automatic diagram axes

POST: s-d-a x x(fcc_al,c)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y x(fcc_al,ni)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a z x(fcc_al,cr)
... the command in full is SET_DIAGRAM_AXIS
POST:
POST: s-a-t-s y y
... the command in full is SET_AXIS_TEXT_STATUS
POST: s-a-t-s x y
... the command in full is SET_AXIS_TEXT_STATUS
POST: s-a-t-s z y
... the command in full is SET_AXIS_TEXT_STATUS
POST:
POST: s-s-s x n 0 0.1
... the command in full is SET_SCALING_STATUS
POST: s-s-s y n 0 1
... the command in full is SET_SCALING_STATUS
POST: s-s-s z n 0 1
... the command in full is SET_SCALING_STATUS
POST:
POST: set-title example 47e
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

# example 47e

2016.05.16 14.45.22  
FEDEMO: C, CR, FE, NI  
T=1373, N=1, P=1E5, X(FCC\_A1,CR)=0.16



```

POST:
POST:
POST:Hit RETURN to continue
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the Cr content in the fcc_a1 phase, in the second ni content
POST: @@ and in the last column the C content of the fcc_a1 phase.
POST: e-sym tab tab5
... the command in full is ENTER_SYMBOL
Variable(s): x(fcc_a1,cr),x(fcc_a1,ni),x(fcc_a1,c)
&
POST: @@ Save the tabulated data on file
POST: tab tab5 fecrnic_1373.tab
... the command in full is TABULATE
POST:
POST:
POST: back
POLY_3: rei,,,,
... the command in full is REINITIATE_MODULE
POLY_3:
POLY_3: s-c t=1373
... the command in full is SET_CONDITION
POLY_3: se-co n=1,p=1e5
... the command in full is SET_CONDITION
POLY_3: se-co x(C)=.01
... the command in full is SET_CONDITION
POLY_3: se-co x(ni)=.001
... the command in full is SET_CONDITION
POLY_3: se-co x(cr)=.01
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 9750 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY_3:
POLY_3: s-a-v 1 x(c) 0 1 .001
... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 x(ni) 0 1 .001
... the command in full is SET_AXIS_VARIABLE
POLY_3: add-in 1,,,
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-co x(cr)=.05
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Using already calculated grid
Found the set of lowest grid points in 0 s
Calculated POLY solution 1 s, total time 1 s
POLY_3: add-in 1,,,
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: se-co x(cr)=.1
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Using already calculated grid
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY_3: add-in 1,,,
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3:
POLY_3: advanced
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: present
Phase name /NONE/: fcc_a1
POLY_3: save tcex47 y
... the command in full is SAVE_WORKSPACES

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

POLY_3: map
Version S mapping is selected

```

Organizing start points

Using ADDED start equilibria

Tie-lines not in the plane of calculation

Generating start point 1  
Generating start point 2  
Generating start point 3  
Generating start point 4  
Generating start point 5  
Generating start point 6

Phase region boundary 1 at: 7.757E-02 1.000E-03  
\*\* CEMENTITE  
FCC\_A1  
Calculated 8 equilibria

Phase region boundary 2 at: 7.757E-02 1.000E-03  
\*\* CEMENTITE  
FCC\_A1  
Calculated 969 equilibria

Phase region boundary 3 at: 5.282E-02 1.000E-03  
FCC\_A1  
\*\* M7C3  
Calculated 15 equilibria

Phase region boundary 4 at: 5.282E-02 1.000E-03  
FCC\_A1  
\*\* M7C3  
Calculated. 694 equilibria

Phase region boundary 5 at: 2.910E-02 6.938E-01  
FCC\_A1  
\*\* FCC\_A1#2  
\*\* M7C3

Phase region boundary 6 at: 2.910E-02 6.938E-01  
FCC\_A1  
FCC\_A1#2  
\*\* M7C3  
Calculated. 95 equilibria

Phase region boundary 7 at: 7.037E-02 6.004E-01  
\*\* CEMENTITE  
FCC\_A1  
FCC\_A1#2  
\*\* M7C3

Phase region boundary 8 at: 1.432E-01 5.581E-01  
CEMENTITE  
FCC\_A1  
\*\* FCC\_A1#2  
Calculated. 214 equilibria

Phase region boundary 9 at: 3.838E-02 7.703E-01  
\*\* CEMENTITE  
FCC\_A1  
\*\* FCC\_A1#2

Phase region boundary 10 at: 3.838E-02 7.703E-01  
FCC\_A1  
\*\* FCC\_A1#2  
Calculated. 78 equilibria  
Terminating at known equilibrium

Phase region boundary 11 at: 3.838E-02 7.703E-01  
\*\* CEMENTITE  
FCC\_A1  
Calculated 156 equilibria

Phase region boundary 12 at: 3.838E-02 7.703E-01  
\*\* CEMENTITE  
FCC\_A1  
FCC\_A1#2  
Calculated. 171 equilibria  
Terminating at known equilibrium

Phase region boundary 13 at: 1.432E-01 5.581E-01  
CEMENTITE  
FCC\_A1  
\*\* M7C3  
Calculated 582 equilibria

Phase region boundary 14 at: 7.104E-02 5.895E-01  
\*\* CEMENTITE  
FCC\_A1  
M7C3  
Calculated 603 equilibria

Phase region boundary 15 at: 7.104E-02 5.895E-01  
FCC\_A1  
\*\* FCC\_A1#2  
M7C3  
Calculated. 106 equilibria  
Terminating at known equilibrium

Phase region boundary 16 at: 2.910E-02 6.938E-01  
FCC\_A1  
\*\* M7C3  
Calculated 707 equilibria

Phase region boundary 17 at: 2.819E-02 1.000E-03  
FCC\_A1  
\*\* M7C3  
Calculated 8 equilibria

Phase region boundary 18 at: 2.819E-02 1.000E-03  
FCC\_A1  
\*\* M7C3  
Calculated. 813 equilibria

Phase region boundary 19 at: 3.066E-02 8.126E-01  
FCC\_A1  
\*\* FCC\_A1#2  
\*\* M7C3

```

Phase region boundary 20 at: 3.066E-02 8.126E-01
  FCC_A1
  FCC_A1#2
  ** M7C3
Calculated. 290 equilibria
Terminating at known equilibrium

Phase region boundary 21 at: 3.066E-02 8.126E-01
  FCC_A1
  ** FCC_A1#2
Calculated 58 equilibria

Phase region boundary 22 at: 3.066E-02 8.126E-01
  FCC_A1
  ** FCC_A1#2
  M7C3
Calculated. 324 equilibria
Terminating at known equilibrium

Phase region boundary 23 at: 3.066E-02 8.126E-01
  FCC_A1
  ** M7C3
Calculated 822 equilibria
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex47\tcex
47.POLY3
CPU time for mapping 12 seconds
POLY_3:
POLY_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POST:
POST: se-d-t n y,,,
... the command in full is SET_DIAGRAM_TYPE
POST:
POST: @@ Enter a table for the calculated data. In the first column put
POST: @@ the Cr content in the fcc_al phase, in the second ni
POST: @@ and in the last column the C content of the fcc_al phase.
POST: e-sym tab tab6
... the command in full is ENTER_SYMBOL
Variable(s): x(fcc_al,cr),x(fcc_al,ni),x(fcc_al,c)
&
POST: se-tit
... the command in full is SET_TITLE
TITLE : Fe-Cr-Ni-C system
POST: s-d-a x x(fcc_al,cr)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y x(fcc_al,ni)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a z x(fcc_al,c)
... the command in full is SET_DIAGRAM_AXIS
POST:
POST: s-a-t-s x n X(Cr)
... the command in full is SET_AXIS_TEXT_STATUS
POST: s-a-t-s y n X(Ni)
... the command in full is SET_AXIS_TEXT_STATUS
POST: s-a-t-s z n X(C)
... the command in full is SET_AXIS_TEXT_STATUS
POST:
POST: @@ Finally, create the 3D-diagram (or .wrl file) by merging data
POST: @@ from the different tables created and saved. This is accomplished
POST: @@ using the command "CREATE_3D_DIAGRAM". Also define the scaling
POST: @@ to be used in the 3D-diagram.
POST: cre BOTH tab6
... the command in full is CREATE_3D_PLOTFILE
The table must contain values for X,Y and Z axis
DEFINED CONSTANTS
  ZERO=0
DEFINED FUNCTIONS AND VARIABLES%
  TEMP_C=T-273.15
DEFINED TABLES
  TAB6=X(FCC_A1,CR), X(FCC_A1,NI), X(FCC_A1,C)
Give TAB filename: /Cancel_to_finish/: fecrc_1373.tab fecrni_1373.tab fecnic_1373.tab fecrnic_1373.tab Cancel_to
Output file: /3Dplot/: tcex47.wrl
X-AXIS SCALING FROM 0.0 TO XMAX /1/: 1
Y-AXIS SCALING FROM 0.0 TO YMAX /1/: 1
TETRAHEDRON DIAGRAM, ZMIN SET 0.0
Z-AXIS SCALING, GIVE ZMAX /2000/: .5

It is possible to combine files by:
Copy Ter.tab+Bin1.tab+Bin2.tab+Bin3.tab Tmp.tab

Processing fecrc_1373.tab
5.287230000000000E-009 <X< 0.1806920000000000
0.000000000000000E+000 <Y< 0.000000000000000E+000
6.987710000000000E-009 <Z< 8.158250000000000E-002

Processing fecrni_1373.tab
0.113628000000000 <X< 0.478622000000000
2.068240000000000E-008 <Y< 0.521377000000000
0.000000000000000E+000 <Z< 0.000000000000000E+000

Processing fecnic_1373.tab
0.000000000000000E+000 <X< 0.000000000000000E+000
1.100300000000000E-008 <Y< 0.968861000000000
2.918660000000000E-002 <Z< 8.158250000000000E-002

Processing crnic_1373.tab
7.671840000000000E-010 <X< 0.481628000000000
0.515960000000000 <Y< 0.968861000000000
1.000000000000000E-012 <Z< 4.498370000000000E-002

Processing fecrnic_1373.tab
2.000000000000000E-002 <X< 0.160000000000000
9.371880000000000E-013 <Y< 0.945434000000000
3.608350000000000E-003 <Z< 7.342520000000000E-002
POST:
POST: se-inter
... the command in full is SET_INTERACTIVE_MODE

```





tcex48

```
AboutMACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex48\tcex48.TCM"SYS: set-echo
SYS: @@
SYS: @@ Scheil solidification with C back diffusion in solid phases and comparison with simple Scheil and equilibrium calculations.
SYS: @@
SYS: @@ Scheil solidification with C back diffusion (ScheiC) in solid phases
SYS: @@ and
SYS: @@ comparison with simple Scheil and equilibrium calculations
SYS: @@
SYS: set-log ex48,,,
SYS: @@ use system command delete old exp files if any
SYS: @@ for unix
SYS: @@ rm *.exp
SYS: @@ for pc
SYS: @del *.exp
Det g?r inte att hitta c:\jenkins\WORKSP~1\THERMO~1\examples\tcex48\*.exp.
SYS: @@
SYS: @@ first do ScheiC by assigning C as fast diffuse element
SYS: @@ plot solidification and microsegregation diagram and save them
SYS: @@ to files
SYS: @@
SYS: go scheil
... the command in full is GOTO_MODULE
SCHEIL: save-file-name tcex48a
SCHEIL: start
... the command in full is START_WIZARD
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
L12_FCC B2_BCC B2_VACANCY
HIGH_SIGMA DICTRA_FCC_A1 REJECTED
Database /TCFE8/: FEDEMO
Current database: Iron Demo Database

VA /- DEFINED
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/: Y
1st alloying element: c 1
2nd alloying element: cr 10
Next alloying element:
Temperature (C) /2000/: 2000
VA /- DEFINED
REINITIATING GES5 .....
... the command in full is DEFINE_ELEMENTS
FE DEFINED
... the command in full is DEFINE_ELEMENTS
C DEFINED
... the command in full is DEFINE_ELEMENTS
CR DEFINED

This database has following phases for the defined system

GAS:G LIQUID:L BCC_A2
CEMENTITE CHI_A12 DIAMOND_FCC_A4
FCC_A1 GRAPHITE HCP_A3
KSI_CARBIDE LAVES_PHASE_C14 M23C6
M3C2 M5C2 M7C3
SIGMA

Reject phase(s) /NONE/: NONE
Restore phase(s): /NONE/: NONE

.....

The following phases are retained in this system:

GAS:G LIQUID:L BCC_A2
CEMENTITE CHI_A12 DIAMOND_FCC_A4
FCC_A1 GRAPHITE HCP_A3
KSI_CARBIDE LAVES_PHASE_C14 M23C6
M3C2 M5C2 M7C3
SIGMA

.....

OK? /Y/: Y
GAS:G REJECTED
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'
'B. Uhrenius (1993-1994), International journal of refractory metals and
hard mater, Vol. 12, pp. 121-127; Molar volumes'
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'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
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'J.-O. Andersson, Calphad, 11 (1987), 271-276; TRITA 0314; C-CR'
'B.-J. Lee, Calphad (1993); revision of Fe-Cr and Fe-Ni liquid'
'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
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'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
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'B.-J. Lee, unpublished revision (1991); C-Cr-Fe-Ni'
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(1986); CR-FE'
'P. Villars and L.D. Calvert (1985). Pearsons handbook of crystallographic
data for intermetallic phases. Metals park, Ohio. American Society for
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'J. Bratberg, Z. Metallkd., Vol 96 (2005), 335-344; Fe-Cr-Mo-C'
```

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'P. Gustafson, TRITA-MAC 342 (1987); CR-FE-W'
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'P. Gustafson, Metall. Trans. A, 19A (1988), 2547-2554; TRITA-MAC 348,
(1987); C-CR-FE-W'
'K. Frisk, Metall. Trans. A, 21A (1990), 2477-2488; TRITA 0409 (1989); CR
-FE-N'
'J-O. Andersson, Calphad, 12 (1988), 9-23; TRITA 0321 (1986); C -FE-MO'
'N. Saunders, COST 507 Report (1998); Cr-Ti'
'B.-J. Lee, estimated parameter 1999'
'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equil., 19 (1998),
441-448; Fe-Ti'
'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
Sigma model'
-OK-
Should any phase have a miscibility gap check? /N/: N
LIQUID PHASE NAME: LIQUID
Fast diffusing components: /NONE/: C
... the command in full is SET_NUMERICAL_LIMITS
... the command in full is COMPUTE_TRANSITION
This command is a combination of CHANGE_STATUS and SET_CONDITION
to calculate directly when a phase may form by releasing one condition.
You must release one of these conditions
T=2273.15, W(C)=1E-2, W(CR)=0.1, P=1E5, N=1 DEGREES OF FREEDOM 0
To form FCC_A1#1 the condition is set to T=1716.48507839
CALCULATING USING NORMAL EQUILIBRIUM CONDITIONS
... the command in full is ADD_INITIAL_EQUILIBRIUM
... the command in full is ADVANCED_OPTIONS
... the command in full is STEP_WITH_OPTIONS
...OK

Phase Region from 1716.48 for:
LIQUID
FCC_A1
Global Check of removing phase at 1.71649E+03
Calculated 3 equilibria

Phase Region from 1716.49 for:
LIQUID
Terminating at 1716.58
Calculated 4 equilibria

Phase Region from 1716.48 for:
LIQUID
FCC_A1
Global test at 1.70848E+03 .... OK
Global test at 1.69848E+03 .... OK
Global test at 1.68848E+03 .... OK
Global test at 1.67848E+03 .... OK
Global test at 1.66848E+03 .... OK
Global test at 1.65848E+03 .... OK
Global test at 1.64848E+03 .... OK
Global test at 1.63848E+03 .... OK
Global test at 1.62848E+03 .... OK
Global test at 1.61848E+03 .... OK
Global check of removing phase at 1.61342E+03
Calculated 106 equilibria

Phase Region from 1613.42 for:
FCC_A1
Calculated 4 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex48\tcex
48a.POLY3

POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

... the command in full is ENTER_SYMBOL
... the command in full is MAKE_EXPERIMENTAL_DATAFI
An EXP file c:\jenkins\WORKSP~1\THERMO~1\examples\tcex48\tcex48a_EQ.EXP
has been created to store the equilibrium solidification results.
... the command in full is READ_WORKSPACES
CALCULATING SCHEEL SOLIDIFICATION
... the command in full is SET_NUMERICAL_LIMITS

T(C) fraction solid

1443.425 0.000000

PHASE REGION:LIQUID + FCC_A1

T(C) fraction solid

1443.331 0.000000
1442.331 0.2475817E-01
1441.331 0.4847108E-01
1440.331 0.7146723E-01
1439.331 0.9377411E-01
1438.331 0.1154198
1437.331 0.1364307
1436.331 0.1568321
1435.331 0.1766476
1434.331 0.1958998
1433.331 0.2146101
1432.331 0.2327987
1431.331 0.2504848
1430.331 0.2676869
1429.331 0.2844222
1428.331 0.3007072
1427.331 0.3165578
1426.331 0.3319888
1425.331 0.3470146
1424.331 0.3616488
1423.331 0.3759043
1422.331 0.3897936
1421.331 0.4033284

```

1420.331	0.4165201
1419.331	0.4293794
1418.331	0.4419167
1417.331	0.4541419
1416.331	0.4660643
1415.331	0.4776932
1414.331	0.4890371
1413.331	0.5001044
1412.331	0.5109030
1411.331	0.5214407
1410.331	0.5317247
1409.331	0.5417621
1408.331	0.5515598
1407.331	0.5611242
1406.331	0.5704616
1405.331	0.5795781
1404.331	0.5884795
1403.331	0.5971714
1402.331	0.6056592
1401.331	0.6139481
1400.331	0.6220433
1399.331	0.6299494
1398.331	0.6376713
1397.331	0.6452135
1396.331	0.6525803
1395.331	0.6597760
1394.331	0.6668048
1393.331	0.6736706
1392.331	0.6803774
1391.331	0.6869287
1390.331	0.6933284
1389.331	0.6995799
1388.331	0.7056866
1387.331	0.7116520
1386.331	0.7174792
1385.331	0.7231714
1384.331	0.7287317
1383.331	0.7341631
1382.331	0.7394684
1381.331	0.7446507
1380.331	0.7497126
1379.331	0.7546568
1378.331	0.7594860
1377.331	0.7642028
1376.331	0.7688097
1375.331	0.7733092
1374.331	0.7777037
1373.331	0.7819955
1372.331	0.7861870
1371.331	0.7902805
1370.331	0.7942781
1369.331	0.7981819
1368.331	0.8019943
1367.331	0.8057171
1366.331	0.8093525
1365.331	0.8129024
1364.331	0.8163688
1363.331	0.8197537
1362.331	0.8230588
1361.331	0.8262861
1360.331	0.8294373
1359.331	0.8325142
1358.331	0.8355186
1357.331	0.8384521
1356.331	0.8413165
1355.331	0.8441132
1354.331	0.8468440
1353.331	0.8495104
1352.331	0.8521139
1351.331	0.8546561
1350.331	0.8571384
1349.331	0.8595622
1348.331	0.8619289
1347.331	0.8642400
1346.331	0.8664968
1345.331	0.8687006
1344.331	0.8708527
1343.331	0.8729544
1342.331	0.8750069
1341.331	0.8770114
1340.331	0.8789691
1339.331	0.8808811
1338.331	0.8827487
1337.331	0.8845728
1336.331	0.8863546
1335.331	0.8880952
1334.331	0.8897955
1333.331	0.8914566
1332.331	0.8930794
1331.331	0.8946650
1330.331	0.8962142
1329.331	0.8977279
1328.331	0.8992071
1327.331	0.9006527
1326.331	0.9020654
1325.331	0.9034461
1324.331	0.9047956
1323.331	0.9061147
1322.331	0.9074042
1321.331	0.9086649
1320.331	0.9098973
1319.331	0.9111023
1318.331	0.9122806
1317.331	0.9134328
1316.331	0.9145596
1315.331	0.9156617
1314.331	0.9167396
1313.331	0.9177939
1312.331	0.9188254
1311.331	0.9198345
1310.331	0.9208217
1309.331	0.9217878
1308.331	0.9227331
1307.331	0.9236583
1306.331	0.9245638
1305.331	0.9254501

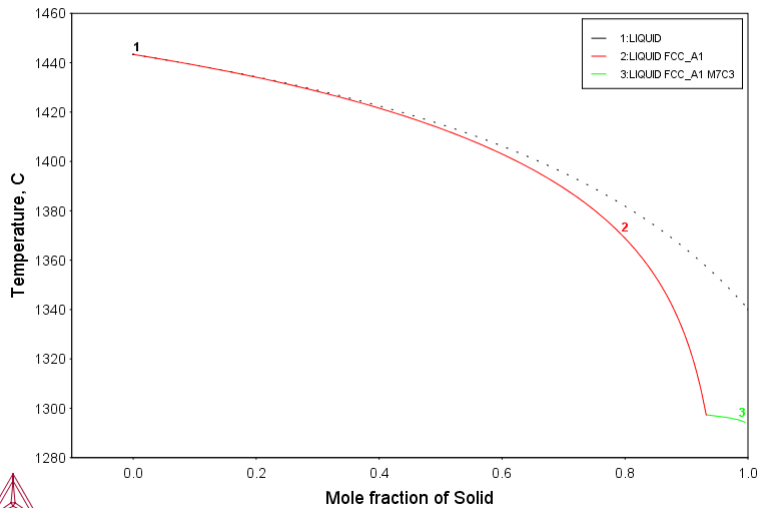
1304.331	0.9263177
1303.331	0.9271671
1302.331	0.9279988
1301.331	0.9288131
1300.331	0.9296105
1299.331	0.9303915
1298.331	0.9311564
1297.363	0.9318915

PHASE REGION:LIQUID + FCC\_A1 + M7C3

T(C)	fraction solid
1297.331	0.9321898
1296.331	0.9644012
1295.331	0.9850907
1294.331	0.9951874

Hint: move the last function to the first equilibrium where it is used

... the command in full is SET\_LABEL\_CURVE\_OPTION  
 ... the command in full is APPEND EXPERIMENTAL DATA  
 2016.05.16.14.48.36  
 FEDEMO: C, CR, FE  
 T=1716.58, W(C)=1E-2, W(CR)=0.1, P=1E5, N=1



... the command in full is APPEND\_EXPERIMENTAL\_DATA

.....

The following axis variables are available

T --- Temperature in Celsius  
 NL/BL --- Mole/mass fraction of liquid  
 NS/BS --- Mole/mass fraction of all solid phases  
 NS(ph)/BS(ph) --- Mole/mass fraction of a solid phase  
 W(ph,el) --- Weight fraction of an element in a phase  
 X(ph,el) --- Mole fraction of an element in a phase  
 Y(ph,el) --- Site fraction of an element in a phase  
 NN(ph,el) --- Distribution of an element in a phases  
 NH/BH --- Heat release and Latent heat per mole/gram  
 CP/BCP --- Apparent heat capacity per mole/gram  
 NV/NV(ph) --- Molar volume of the system or a phase  
 DS/DS(ph) --- Average density of the system or a phase  
 BT --- Apparent volumetric TEC of the system

"el" and "ph" are name of element and phase, respectively  
 "\*" can be used as a wild character for "el" and "ph"

.....

POST:Hit RETURN to continue

POST: make tcex48a.exp y

... the command in full is MAKE\_EXPERIMENTAL\_DATAFI

POST:

POST: set-dia-ax x ns(fcc\_a1)

... the command in full is SET\_DIAGRAM\_AXIS

POST: set-dia-ax y w(fcc\_a1,cr)

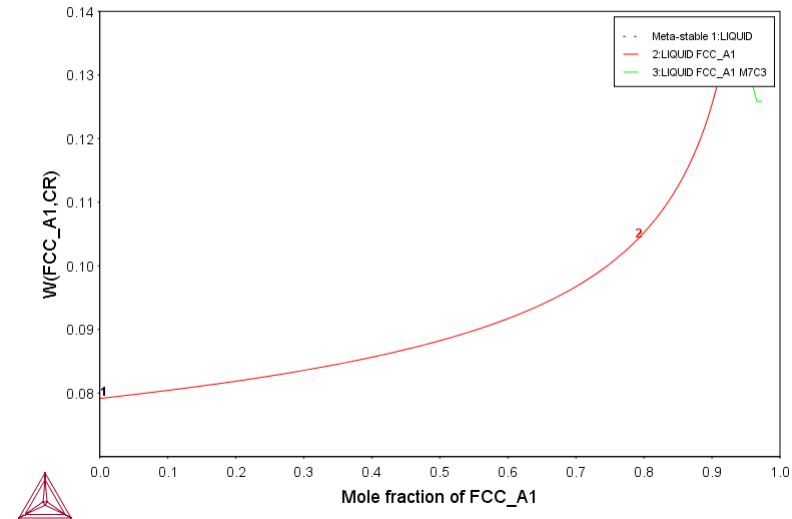
... the command in full is SET\_DIAGRAM\_AXIS

POST:

POST: plot,,,,,

... the command in full is PLOT\_DIAGRAM

2016.05.16.14.48.38  
 FEDEMO: C, CR, FE  
 T=1716.58, W(C)=1E-2, W(CR)=0.1, P=1E5, N=1



```

POST:Hit RETURN to continue
POST:
POST:
POST: make tcex48b.exp y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST:
POST: back
SCHEIL: @@
SCHEIL: @@ Ignore back diffusion of C in solids and do Scheil with the same alloy
SCHEIL: @@ by choosing option 3 from the Scheil simulation option list.
SCHEIL: @@ also plot solidification and microsegregation diagrams
SCHEIL: @@ save them to files
SCHEIL: @@
SCHEIL:
SCHEIL: save-file-name tcex48b
SCHEIL: start
... the command in full is START_WIZARD
Database /TCFE8/: FEDEMO
Major element or alloy: fe
Composition input in mass (weight) percent? /Y/: Y
1st alloying element: c 1
2nd alloying element: cr 10
Next alloying element:
Temperature (C) /2000/: 1700
VA          /-  DEFINED
REINITIATING GES5 .....
... the command in full is DEFINE_ELEMENTS
FE  DEFINED
... the command in full is DEFINE_ELEMENTS
C   DEFINED
... the command in full is DEFINE_ELEMENTS
CR  DEFINED
  
```

This database has following phases for the defined system

GAS:G	LIQUID:L	BCC_A2
CEMENTITE	CHI_A12	DIAMOND_FCC_A4
FCC_A1	GRAPHITE	HCP_A3
KSI_CARBIDE	LAVES_PHASE_C14	M23C6
M3C2	M5C2	M7C3
SIGMA		

Reject phase(s) /NONE/: NONE  
 Restore phase(s): /NONE/: NONE

```

.....

The following phases are retained in this system:

GAS:G          LIQUID:L          BCC_A2
CEMENTITE      CHI_A12        DIAMOND_FCC_A4
FCC_A1         GRAPHITE       HCP_A3
KSI_CARBIDE    LAVES_PHASE_C14 M23C6
M3C2           M5C2           M7C3
SIGMA
  
```

```

OK? /Y/: Y
GAS:G REJECTED
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....
  
```

List of references for assessed data

'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317 -425'  
 'B. Uhrenius (1993-1994), International journal of refractory metals and hard mater, Vol. 12, pp. 121-127; Molar volumes'  
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 'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89; Molar volumes'  
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 'J.-O. Andersson, Calphad, 11 (1987), 271-276; TRITA 0314; C-CR'  
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```

'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
-FE'
'X.-G. Lu, Thermo-Calc Software AB, Sweden,2006; Molar volumes'
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'J-O. Andersson, Metall. Trans. A, 19A (1988), 627-636 TRITA 0207 (1986);
C-CR-FE'
'J-O. Andersson and B. Sundman, Calphad, 11 (1987), 83-92; TRITA 0270
(1986); CR-FE'
'P. Villars and L.D. Calvert (1985). Pearsons handbook of crystallographic
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'J-O. Andersson, Metall. Trans. A, 19A (1988), 1385-1394; TRITA 0322
(1986); CR-FE-MO'
'C. Qiu, ISIJ International, 32 (1992), 1117-1127; C-Cr-Fe-Mo'
'P. Gustafson, Metall. Trans. A, 19A (1988), 2547-2554; TRITA-MAC 348,
(1987); C-CR-FE-W'
'K. Frisk, Metall. Trans. A, 21A (1990), 2477-2488; TRITA 0409 (1989); CR
-FE-N'
'J-O. Andersson, Calphad, 12 (1988), 9-23; TRITA 0321 (1986); C -FE-MO'
'N. Saunders, COST 507 Report (1998); Cr-Ti'
'B.-J. Lee, estimated parameter 1999'
'L.F.S. Dumitrescu, M. Hillert and N. Saunders, J. Phase Equil., 19 (1998),
441-448; Fe-Ti'
'B. Sundman et al., Report EUR 20315, Contract No 7210-PR/050, 2002; New
Sigma model'
-OK-
Should any phase have a miscibility gap check? /N/: N
Fast diffusing components: /NONE/: NONE
... the command in full is SET_NUMERICAL_LIMITS
... the command in full is COMPUTE_TRANSITION
This command is a combination of CHANGE_STATUS and SET_CONDITION
to calculate directly when a phase may form by releasing one condition.
You must release one of these conditions
T=1973.15, W(C)=1E-2, W(CR)=0.1, P=1E5, N=1 DEGREES OF FREEDOM 0
To form FCC_A1#1 the condition is set to T=1716.48507839
CALCULATING USING NORMAL EQUILIBRIUM CONDITIONS
... the command in full is ADD_INITIAL_EQUILIBRIUM
... the command in full is ADVANCED_OPTIONS
... the command in full is STEP_WITH_OPTIONS
...OK

Phase Region from 1716.48 for:
LIQUID
FCC_A1
Global check of removing phase at 1.71649E+03
Calculated 3 equilibria

Phase Region from 1716.49 for:
LIQUID
Terminating at 1716.58
Calculated 4 equilibria

Phase Region from 1716.48 for:
LIQUID
FCC_A1
Global test at 1.70848E+03 .... OK
Global test at 1.69848E+03 .... OK
Global test at 1.68848E+03 .... OK
Global test at 1.67848E+03 .... OK
Global test at 1.66848E+03 .... OK
Global test at 1.65848E+03 .... OK
Global test at 1.64848E+03 .... OK
Global test at 1.63848E+03 .... OK
Global test at 1.62848E+03 .... OK
Global test at 1.61848E+03 .... OK
Global check of removing phase at 1.61342E+03
Calculated 106 equilibria

Phase Region from 1613.42 for:
FCC_A1
Calculated 4 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex48\tcex
48b.POLY3

POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

... the command in full is ENTER_SYMBOL
... the command in full is MAKE_EXPERIMENTAL_DATAFI
An EXP file c:\jenkins\WORKSP~1\THERMO~1\examples\tcex48\tcex48b_EQ.EXP
has been created to store the equilibrium solidification results.
... the command in full is READ_WORKSPACES
CALCULATING SCHEIL SOLIDIFICATION
... the command in full is SET_NUMERICAL_LIMITS

T(C) fraction solid

1443.425 0.000000

PHASE REGION:LIQUID + FCC_A1

T(C) fraction solid

1443.331 0.9380064E-04
1442.331 0.2475714E-01
1441.331 0.4847007E-01
1440.331 0.7128104E-01
1439.331 0.9323546E-01
1438.331 0.1143759
1437.331 0.1347424
1436.331 0.1543724
1435.331 0.1733012
1434.331 0.1915621
1433.331 0.2091864
1432.331 0.2262034
1431.331 0.2426409
1430.331 0.2585253
1429.331 0.2738811
1428.331 0.2887318
1427.331 0.3030994

```

1426.331	0.3170049
1425.331	0.3304680
1424.331	0.3435074
1423.331	0.3561409
1422.331	0.3683853
1421.331	0.3802566
1420.331	0.3917699
1419.331	0.4029396
1418.331	0.4137794
1417.331	0.4243022
1416.331	0.4345205
1415.331	0.4444459
1414.331	0.4540898
1413.331	0.4634626
1412.331	0.4725747
1411.331	0.4814356
1410.331	0.4900547
1409.331	0.4984408
1408.331	0.5066022
1407.331	0.5145470
1406.331	0.5222829
1405.331	0.5298172
1404.331	0.5371570
1403.331	0.5443089
1402.331	0.5512795
1401.331	0.5580748
1400.331	0.5647007
1399.331	0.5711630
1398.331	0.5774669
1397.331	0.5836177
1396.331	0.5896203
1395.331	0.5954796
1394.331	0.6012001
1393.331	0.6067863
1392.331	0.6122422
1391.331	0.6175721
1390.331	0.6227797
1389.331	0.6278689
1388.331	0.6328432
1387.331	0.6377061
1386.331	0.6424610
1385.331	0.6471111
1384.331	0.6516594
1383.331	0.6561089
1382.331	0.6604625
1381.331	0.6647229
1380.331	0.6688929
1379.331	0.6729750
1378.331	0.6769717
1377.331	0.6808852
1376.331	0.6847181
1375.331	0.6884724
1374.331	0.6921504
1373.331	0.6957540
1372.331	0.6992854
1371.331	0.7027464
1370.331	0.7061389
1369.331	0.7094647
1368.331	0.7127256
1367.331	0.7159233
1366.331	0.7190593
1365.331	0.7221353
1364.331	0.7251527
1363.331	0.7281132
1362.331	0.7310181
1361.331	0.7338687
1360.331	0.7366665
1359.331	0.7394127
1358.331	0.7421087
1357.331	0.7447556
1356.331	0.7473545
1355.331	0.7499068
1354.331	0.7524134
1353.331	0.7548755
1352.331	0.7572940
1351.331	0.7596701
1350.331	0.7620047
1349.331	0.7642988
1348.331	0.7665533
1347.331	0.7687690
1346.331	0.7709470
1345.331	0.7730879
1344.331	0.7751928
1343.331	0.7772623
1342.331	0.7792972
1341.331	0.7812983
1340.331	0.7832664
1339.331	0.7852022
1338.331	0.7871063
1337.331	0.7889794
1336.331	0.7908223
1335.331	0.7926355
1334.331	0.7944197
1333.331	0.7961755
1332.331	0.7979034
1331.331	0.7996042
1330.331	0.8012782
1329.331	0.8029261
1328.331	0.8045484
1327.331	0.8061457
1326.331	0.8077183
1325.331	0.8092669
1324.331	0.8107920
1323.331	0.8122939
1322.331	0.8137731
1321.331	0.8152301
1320.331	0.8166654
1319.331	0.8180793
1318.331	0.8194723
1317.331	0.8208447
1316.331	0.8221970
1315.331	0.8235296
1314.331	0.8248428
1313.331	0.8261370
1312.331	0.8274126
1311.331	0.8286698



1310.331	0.8299091
1309.331	0.8311309
1308.331	0.8323353
1307.331	0.8335227
1306.331	0.8346935
1305.331	0.8358480
1304.331	0.8369864
1303.331	0.8381091
1302.331	0.8392162
1301.331	0.8403082
1300.331	0.8413853
1299.331	0.8424477
1298.331	0.8434958
1297.331	0.8445297
1296.331	0.8455497
1295.331	0.8465561
1294.331	0.8475491
1293.331	0.8485289
1292.331	0.8494958
1291.331	0.8504500
1290.331	0.8513917
1289.331	0.8523211
1288.331	0.8532384
1287.331	0.8541439
1286.331	0.8550378
1285.331	0.8559202
1284.331	0.8567913
1283.613	0.8574103

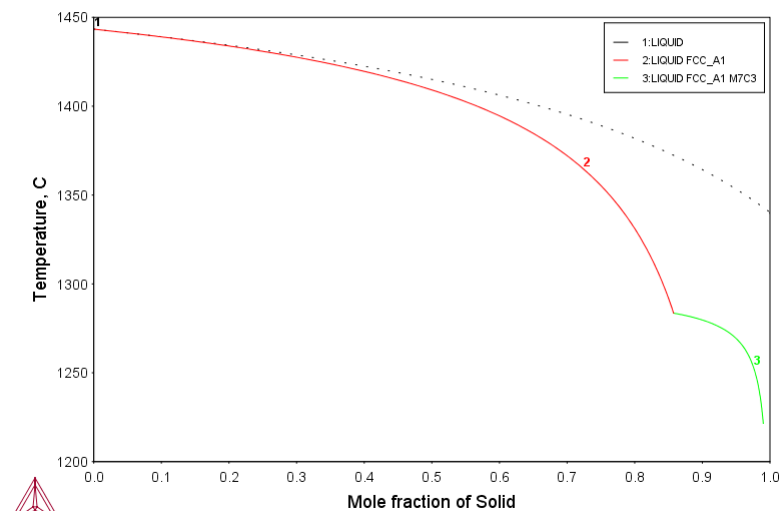
PHASE REGION:LIQUID + FCC\_A1 + M7C3

T(C)	fraction solid
1283.581	0.8575876
1282.581	0.8709413
1281.581	0.8824023
1280.581	0.8923216
1279.581	0.9009710
1278.581	0.9085643
1277.581	0.9152712
1276.581	0.9212283
1275.581	0.9265464
1274.581	0.9313162
1273.581	0.9356128
1272.581	0.9394983
1271.581	0.9430252
1270.581	0.9462374
1269.581	0.9491724
1268.581	0.9518620
1267.581	0.9543337
1266.581	0.9566111
1265.581	0.9587145
1264.581	0.9606618
1263.581	0.9624685
1262.581	0.9641482
1261.581	0.9657129
1260.581	0.9671731
1259.581	0.9685382
1258.581	0.9698165
1257.581	0.9710154
1256.581	0.9721416
1255.581	0.9732011
1254.581	0.9741990
1253.581	0.9751403
1252.581	0.9760293
1251.581	0.9768699
1250.581	0.9776656
1249.581	0.9784196
1248.581	0.9791350
1247.581	0.9798144
1246.581	0.9804603
1245.581	0.9810748
1244.581	0.9816600
1243.581	0.9822179
1242.581	0.9827501
1241.581	0.9832582
1240.581	0.9837437
1239.581	0.9842081
1238.581	0.9846524
1237.581	0.9850780
1236.581	0.9854858
1235.581	0.9858768
1234.581	0.9862521
1233.581	0.9866124
1232.581	0.9869586
1231.581	0.9872915
1230.581	0.9876116
1229.581	0.9879197
1228.581	0.9882164
1227.581	0.9885023
1226.581	0.9887779
1225.581	0.9890437
1224.581	0.9893001
1223.581	0.9895477
1222.581	0.9897868
1221.581	0.9900178

Hint: move the last function to the first equilibrium where it is used

... the command in full is SET\_LABEL\_CURVE\_OPTION  
 ... the command in full is APPEND\_EXPERIMENTAL\_DATA

2016.05.16.14.48.45  
 FEDEMO: C, CR, FE  
 T=1716.58, W(C)=1E-2, W(CR)=0.1, P=1E5, N=1



... the command in full is APPEND\_EXPERIMENTAL\_DATA

The following axis variables are available

T --- Temperature in Celsius  
 NL/BL --- Mole/mass fraction of liquid  
 NS/BS --- Mole/mass fraction of all solid phases  
 NS(ph)/BS(ph) --- Mole/mass fraction of a solid phase  
 W(ph,el) --- Weight fraction of an element in a phase  
 X(ph,el) --- Mole fraction of an element in a phase  
 Y(ph,el) --- Site fraction of an element in a phase  
 NN(ph,el) --- Distribution of an element in a phases  
 NH/BH --- Heat release and Latent heat per mole/gram  
 CP/BCP --- Apparent heat capacity per mole/gram  
 NV/NV(ph) --- Molar volume of the system or a phase  
 DS/DS(ph) --- Average density of the system or a phase  
 BT --- Apparent volumetric TEC of the system

"el" and "ph" are name of element and phase, respectively  
 "\*" can be used as a wild character for "el" and "ph"

POST:Hit RETURN to continue

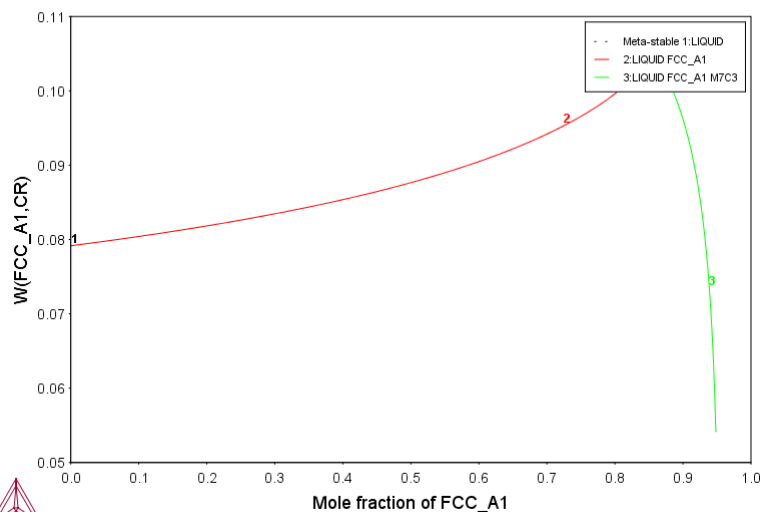
POST: make tcex48c.exp y  
 ... the command in full is MAKE\_EXPERIMENTAL\_DATAFI

POST: set-dia-ax x ns(fcc\_al)  
 ... the command in full is SET\_DIAGRAM\_AXIS

POST: set-dia-ax y w(fcc\_al,cr)  
 ... the command in full is SET\_DIAGRAM\_AXIS

POST:  
 POST: plot,,,,,  
 ... the command in full is PLOT DIAGRAM

2016.05.16.14.48.48  
 FEDEMO: C, CR, FE  
 T=1716.58, W(C)=1E-2, W(CR)=0.1, P=1E5, N=1



POST: make tcex48d.exp y  
 ... the command in full is MAKE\_EXPERIMENTAL\_DATAFI  
 POST: back  
 SCHEIL:Hit RETURN to continue  
 SCHEIL: @@ calculate simple equilibrium solidification of the same alloy  
 SCHEIL: @@ and compare the results with those of Scheil and ScheiC  
 SCHEIL: go p-3  
 ... the command in full is GOTO\_MODULE  
 POLY\_3: read tcex48b  
 ... the command in full is READ\_WORKSPACES  
 POLY\_3: list-condition  
 ... the command in full is LIST CONDITIONS  
 T=1716.58, W(C)=1E-2, W(CR)=0.1, P=1E5, N=1  
 DEGREES OF FREEDOM 0

```

POLY_3: list-equilibrium
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
Output from POLY-3, equilibrium =      1, label A0 , database: FEDEMO

Conditions:
T=1716.58, W(C)=1E-2, W(CR)=0.1, P=1E5, N=1
DEGREES OF FREEDOM 0

Temperature 1716.58 K ( 1443.43 C), Pressure 1.000000E+05
Number of moles of components 1.02132E-02, Mass in grams 4.94687E-01
Total Gibbs energy -9.92311E+02, Enthalpy 6.48245E+02, Volume 7.34133E-08

Component      Moles      W-Fraction Activity Potential Ref.stat
C               1.6474E-03   3.9998E-02 4.6838E-02 -4.3689E+04 SER
CR              9.0314E-04   9.4928E-02 2.0203E-04 -1.2142E+05 SER
FE              7.6627E-03   8.6507E-01 1.3719E-03 -9.4078E+04 SER

LIQUID          Status ENTERED   Driving force 0.0000E+00
Moles 9.7543E-03, Mass 4.7227E-01, Volume fraction 9.5694E-01 Mass fractions:
FE 8.66714E-01 CR 9.31259E-02 C 4.01602E-02

FCC_A1          Status ENTERED   Driving force 0.0000E+00
Moles 3.1121E-04, Mass 1.6266E-02, Volume fraction 3.1001E-02 Mass fractions:
FE 9.28665E-01 CR 5.36480E-02 C 1.76870E-02

M7C3           Status ENTERED   Driving force 0.0000E+00
Moles 1.4776E-04, Mass 6.1527E-03, Volume fraction 1.2058E-02 Mass fractions:
FE 5.71093E-01 CR 3.42373E-01 C 8.65339E-02
POLY_3:Hit RETURN to continue
POLY_3:
POLY_3: reinit
... the command in full is REINITIATE MODULE
POLY_3: set-condition t=1717.15 w(cr)=0.1 w(c)=0.01 p=1e5 n=1
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Global equilibrium calculation turned off, you can turn it on with
ADVANCED_OPTIONS GLOBAL_MINIMIZATION Y,,,,,,,,,
31 ITS, CPU TIME USED 0 SECONDS
POLY_3: set-ax-var 1 t 500 1717.15 10
... the command in full is SET_AXIS_VARIABLE
POLY_3: advanced
... the command in full is ADVANCED_OPTIONS
Which option? /STEP_AND_MAP/: break-condition
Break condition: np(liquid)=0
POLY_3: save tcex48c y
... the command in full is SAVE_WORKSPACES
POLY_3: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, trying to add one          0
Step will start from axis value 1717.15

Phase Region from 1717.15 for:
LIQUID
Calculated 4 equilibria

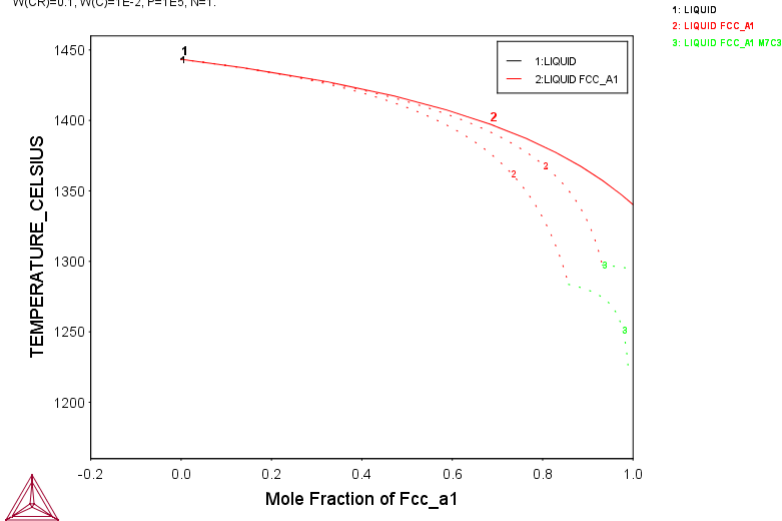
Phase Region from 1716.48 for:
LIQUID
FCC_A1
Calculated 13 equilibria

Phase Region from 1613.42 for:
FCC_A1
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex48\tcex
48c.POLY3
POLY_3: post
POST: @@ define a function to get amount of solids
POST: ent fun fs=1-np(liquid);
... the command in full is ENTER_SYMBOL
POST: @@ plot solidification diagram
POST: set-dia-ax x fs
... the command in full is SET_DIAGRAM_AXIS
POST: set-dia-ax y t-c
... the command in full is SET_DIAGRAM_AXIS
POST: append-exp y tcex48a tcex48c 0; 1; 0; 1;
... the command in full is APPEND_EXPERIMENTAL_DATA
POST: set-ax-text x n
... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Mole Fraction of Fcc_al
POST: set-scaling-status y n 1160 1460
POST: set-title example 48e
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

example 48e

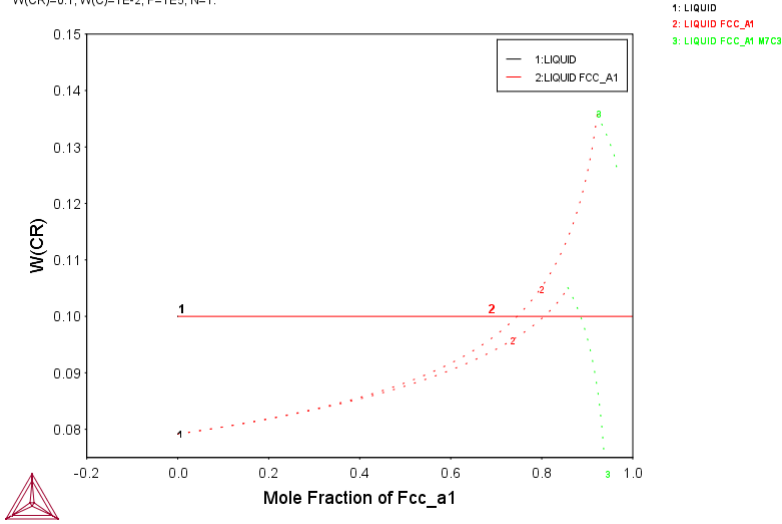
2016.05.16.14.48.50  
FEDEMO: C, CR, FE  
W(CR)=0.1, W(C)=1E-2, P=1E5, N=1.



```
POST:
POST:Hit RETURN to continue
POST:
POST: @@ plot microsegregation which represent the composition profile
POST: @@ of the solid. For equilibrium solidification
POST: @@ there is no solute segregation and the composition of
POST: @@ solidified solid is uniform.
POST: set-dia-ax x fs
... the command in full is SET_DIAGRAM_AXIS
POST: set-dia-ax y w(cr)
... the command in full is SET_DIAGRAM_AXIS
POST: append-exp y tcex48b tcex48d 0; 1; 0; 1;
... the command in full is APPEND_EXPERIMENTAL_DATA
POST: set-ax-text x n
... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Mole Fraction of Fcc_a1
POST: set-scaling y n 0.075 0.15
... the command in full is SET_SCALING_STATUS
POST: set-title example 48f
POST:
POST: plot
... the command in full is PLOT DIAGRAM
```

example 48f

2016.05.16.14.48.50  
FEDEMO: C, CR, FE  
W(CR)=0.1, W(C)=1E-2, P=1E5, N=1.



```
POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:
```

```

AboutMACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex49\tcex49.TCM" set-echo
SYS: @@
SYS: @@ Quasichemical Model via GES
SYS: @@
SYS: @@ Example showing entering parameter for FACT quasichemical liquid model
SYS: @@ and calculating the sulfur activity
SYS:
SYS: set-log ex49,,,
SYS:
SYS: go gibbs
... the command in full is GOTO_MODULE
GIBBS ENERGY SYSTEM version 5.2
GES: ent-el /- VA CU S
... the command in full is ENTER_ELEMENT
THERMODYNAMIC DATABASE module
Current database: Steels/Fe-Alloys v8.0

VA DEFINED
L12 FCC B2 BCC B2_VACANCY
HIGH_SIGMA DICTRA_FCC_A1 REJECTED
GES: am_el_d /- ELECTRON_GAS 0.0000E+00 0.0000E+00 0.0000E+00 1
... the command in full is AMEND_ELEMENT_DATA
GES: am_el_d VA VACUUM 0.0000E+00 0.0000E+00 0.0000E+00 1
... the command in full is AMEND_ELEMENT_DATA
GES: am_el_d CU FCC_A1 6.3546E+01 5.0041E+03 3.3150E+01 1
... the command in full is AMEND_ELEMENT_DATA
GES: am_el_d S FC_ORTHORHOMBIC 3.2066E+01 0.0000E+00 0.0000E+00 1
... the command in full is AMEND_ELEMENT_DATA
GES:
GES:
GES: @@ The quasichemical model requires species entered with the
GES: @@ stoichiometry. The factor 2/ZZ is needed
GES: @@ for the pure elements and 1/ZZ for the compounds.
GES: @@ For Cu ZZ=0.9294 and 2/ZZ_Cu=2.15193
GES: @@ For S ZZ=1.8366 and 2/ZZ_S=1.08897
GES: @@ For CuS the stoichiometries are thus 1/ZZ_Cu=1.07596 and
GES: @@ 1/ZZ_S=0.54448
GES:
GES: enter-specie CUQ CU2.15193
... the command in full is ENTER_SPECIES
GES: enter-specie CUQS CU1.07596S0.54448
... the command in full is ENTER_SPECIES
GES: enter-specie S2 S2
... the command in full is ENTER_SPECIES
GES: enter-specie SQ S1.08897
... the command in full is ENTER_SPECIES
GES:
GES:
GES: @@ The Gibbs energy difference between FCC-Cu and quasichemical liquid-Cu
GES:
GES: ent-sym fun GQCU 2.98150E+02 +16547-7.6815*T; 6.00000E+03 N
... the command in full is ENTER_SYMBOL
GES:
GES:
GES: @@ The Gibbs energy difference between GAS-S and quasichemical liquid-S
GES:
GES: ent-sym fun GQS 2.98150E+02 -65357+165.396*T-13.513*T*LN(T);
... the command in full is ENTER_SYMBOL
HIGH TEMPERATURE LIMIT /6000/: 6.00000E+03 N
GES:
GES:
GES:
GES: @@ Gibbs energies for the pure elements and gases referred 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+0.54448*GSSLIQ ; 6.00000E+03 N
GES:
GES:
GES: @@ The stoichiometry parameter for pure S is 2/ZZ
GES:
GES: ent-param VK(QUASI,SQ;0) 2.98150E+02 1.8366; 6.00000E+03 N
... the command in full is ENTER_PARAMETER
VK(QUASI,SQ;0)
GES:
GES: @@ The energy parameter for pure S (factor is 2/VK)
GES:
GES: ent-param G(QUASI,SQ;0) 2.98150E+02 +1.08897*GSSLIQ ;
... the command in full is ENTER_PARAMETER
G(QUASI,SQ;0)-1.08897 G(FC_ORTHORHOMBIC,S;0)
HIGH TEMPERATURE LIMIT /6000/: 6.00000E+03 N
GES:
GES: @@ The mixing terms
GES:
GES: ent-param G(QUASI,CUQ,CUQS;0) 2.98150E+02 -82768; 6.00000E+03 N
... the command in full is ENTER_PARAMETER
G(QUASI,CUQ,CUQS;0)
GES: ent-param G(QUASI,CUQ,CUQS;1) 2.98150E+02 -32070; 6.00000E+03 N
... the command in full is ENTER_PARAMETER
G(QUASI,CUQ,CUQS;1)
GES: ent-param G(QUASI,CUQ,CUQS;2) 2.98150E+02 68734; 6.00000E+03 N
... the command in full is ENTER_PARAMETER
G(QUASI,CUQ,CUQS;2)
GES: ent-param G(QUASI,CUQ,CUQS;3) 2.98150E+02 -84194+50*T;
... the command in full is ENTER_PARAMETER
G(QUASI,CUQ,CUQS;3)
HIGH TEMPERATURE LIMIT /6000/: 6.00000E+03 N
GES: ent-param G(QUASI,CUQ,CUQS;4) 2.98150E+02 -43638; 6.00000E+03 N
... the command in full is ENTER_PARAMETER
G(QUASI,CUQ,CUQS;4)
GES: ent-param G(QUASI,CUQ,CUQS;5) 2.98150E+02 +20*T; 6.00000E+03 N
... the command in full is ENTER_PARAMETER
G(QUASI,CUQ,CUQS;5)
GES:
GES:
GES: @@ This command makes the entropy calculation according to
GES: @@ FACT quasichemical model
GES:
GES: amend-phase-description QUASI quasi-fact00
GES:
GES:
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?:

```

10UTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT DATE 2016- 5-16  
FROM DATABASE: User data 2016.05.16

ALL DATA IN SI UNITS  
FUNCTIONS VALID FOR 298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

ELEMENT	STABLE	ELEMENT	REFERENCE	MASS	H298-H0	S298
-1	/-	ELECTRON	_GAS	0.0000E+00	0.0000E+00	0.0000E+00
0	VA	VACUUM		0.0000E+00	0.0000E+00	0.0000E+00
1	CU	FCC_A1		6.3546E+01	5.0041E+03	3.3150E+01
2	S	FC_ORTHORHOMBIC		3.2066E+01	0.0000E+00	0.0000E+00

SPECIES	STOICHIOMETRY
1 CU	CU
2 CUQ	CU2.15193
3 CUQS	CU1.07596S0.54448
4 S	S
5 S2	S2
6 SQ	S1.08897
7 VA	VA

GAS  
 CONSTITUENTS: S2  
 $G(\text{GAS}, \text{S2}; 0) - 2 \ G(\text{FC\_ORTHORHOMBIC}, \text{S}; 0) = +\text{GS2GAS} + \text{RTLNP}$

QUASI  
 \$ QUASICHEMICAL-FACT00 ENTROPY CONTRIBUTION  
 CONSTITUENTS: CUQ, CUQS, SQ  
 $\text{VK}(\text{QUASI}, \text{CUQ}; 0) = +.9294$   
 $G(\text{QUASI}, \text{CUQ}; 0) - 2.15193 \ G(\text{FCC\_A1}, \text{CU}; 0) = +2.15193 * \text{GCULIQ} + 2.15193 * \text{GQCU}$   
 $G(\text{QUASI}, \text{CUQS}; 0) - 1.07596 \ G(\text{FCC\_A1}, \text{CU}; 0) - 0.54448 \ G(\text{FC\_ORTHORHOMBIC}, \text{S}; 0) =$   
 $+1.07596 * \text{GCULIQ} + 1.075963 * \text{GQCU} + .54448 * \text{GSSLIQ}$   
 $\text{VK}(\text{QUASI}, \text{SQ}; 0) = +1.8366$   
 $G(\text{QUASI}, \text{SQ}; 0) - 1.08897 \ G(\text{FC\_ORTHORHOMBIC}, \text{S}; 0) = +1.08897 * \text{GSSLIQ}$   
 \$ Binary excess model Legendre with CUQ as independent  
 $L(\text{QUASI}, \text{CUQ}, \text{CUQS}; 0) = -82768$   
 $L(\text{QUASI}, \text{CUQ}, \text{CUQS}; 1) = -32070$   
 $L(\text{QUASI}, \text{CUQ}, \text{CUQS}; 2) = +68734$   
 $L(\text{QUASI}, \text{CUQ}, \text{CUQS}; 3) = -84194 + 50 * T$   
 $L(\text{QUASI}, \text{CUQ}, \text{CUQS}; 4) = -43638$   
 $L(\text{QUASI}, \text{CUQ}, \text{CUQS}; 5) = +20 * T$

FCC A1  
 ADDITIONAL CONTRIBUTION FROM MAGNETIC ORDERING  
 Magnetic function below Curie Temperature  
 $+1.860338755 * \text{TAO}^{**}(-1) - .17449124 * \text{TAO}^{**}3 - .00775516624 * \text{TAO}^{**}9$   
 $- .0017449124 * \text{TAO}^{**}15$   
 Magnetic function above Curie Temperature  
 $- .0426902268 * \text{TAO}^{**}(-5) - .001352453 * \text{TAO}^{**}(-15)$   
 $- 2.84601512 \text{E} - 04 * \text{TAO}^{**}(-25)$   
 CONSTITUENTS: CU  
 $G(\text{FCC\_A1}, \text{CU}; 0) - G(\text{FCC\_A1}, \text{CU}; 0) = 298.15 < T < 3200.00: +\text{GHSERCU}$

SYMBOL	STATUS	VALUE/FUNCTION
1 R	80000000	8.3145100E+00
2 RTLNP	20000000	+R*T*LN(1E-05*P)
103 GQCU	20000000	+16547-7.6815*T
104 GQS	20000000	-65357+165.396*T-13.513*T*LN(T)
105 GHSERCU	20000000	$298.15 < T < 1358.02: -7770.458 + 130.485403 * T - 24.112392 * T * \text{LN}(T)$ $- .00265684 * T^{**}2 + 1.29223 \text{E} - 07 * T^{**}3 + 52478 * T^{**}(-1)$ $1358.02 < T < 3200.00: -13542.33 + 183.804197 * T - 31.38 * T * \text{LN}(T)$ $+ 3.64643 \text{E} + 29 * T^{**}(-9)$
106 GS2GAS	20000000	$298.15 < T < 1000.00: +117374.548 + 2.98629558 * T - 34.09678 * T * \text{LN}(T)$ $- .002325464 * T^{**}2 + 1.85480167 \text{E} - 07 * T^{**}3 + 128593.6 * T^{**}(-1)$ $1000.00 < T < 3400.00: +117352.438 + 2.50383258 * T - 34.04744 * T * \text{LN}(T)$ $- .0021150245 * T^{**}2 + 9.16602333 \text{E} - 08 * T^{**}3 + 175718.45 * T^{**}(-1)$ $3400.00 < T < 6000.00: +124361.091 + 14.5182895 * T - 36.1923 * T * \text{LN}(T)$ $- 5.930925 \text{E} - 04 * T^{**}2 - 7.54259333 \text{E} - 09 * T^{**}3 - 7484105 * T^{**}(-1)$
107 GSSLIQ	20000000	$298.15 < T < 388.36: -4001.549 + 77.889686 * T - 15.504 * T * \text{LN}(T) - .018629 * T^{**}2$ $- 2.4942 \text{E} - 07 * T^{**}3 - 113945 * T^{**}(-1)$ $388.36 < T < 428.15: -5285183.35 + 118449.585 * T - 19762.4 * T * \text{LN}(T)$ $+ 32.79275 * T^{**}2 - .0102214167 * T^{**}3 + 2.646735 \text{E} + 08 * T^{**}(-1)$ $428.15 < T < 432.25: -8174995.23 + 319914.078 * T - 57607.3 * T * \text{LN}(T)$ $+ 135.3045 * T^{**}2 - .0529973333 * T^{**}3$ $432.25 < T < 453.15: -219408.801 + 7758.83993 * T - 1371.85 * T * \text{LN}(T)$ $+ 2.845035 * T^{**}2 - .00101380333 * T^{**}3$ $453.15 < T < 717.00: +92539.872 - 1336.36627 * T + 202.958 * T * \text{LN}(T)$ $- .2531915 * T^{**}2 + 5.18835 \text{E} - 05 * T^{**}3 - 8202200 * T^{**}(-1)$ $717.00 < T < 1300.00: -6889.972 + 176.35482 * T - 32 * T * \text{LN}(T)$
108 GCULIQ	20000000	$298.15 < T < 1358.02: +12964.84 - 9.510243 * T - 5.83932 \text{E} - 21 * T^{**}7 + \text{GHSERCU}$ $1358.02 < T < 3200.00: +13495.4 - 9.920463 * T - 3.64643 \text{E} + 29 * T^{**}(-9) + \text{GHSERCU}$

GES:  
 GES:Hit RETURN to continue  
 GES: go p-3  
 ... the command in full is GOTO\_MODULE

POLY version 3.32

POLY\_3:  
 POLY\_3:  
 POLY\_3:  
 POLY\_3: l-st ph  
 ... the command in full is LIST\_STATUS  
 \*\*\* STATUS FOR ALL PHASES  

PHASE	STATUS	DRIVING FORCE	MOLES
FCC A1	ENTERED	0.000000E+00	0.000000E+00
QUASI	ENTERED	0.000000E+00	0.000000E+00
GAS	ENTERED	0.000000E+00	0.000000E+00

 POLY\_3: c-st p \*=sus  
 ... the command in full is CHANGE\_STATUS  
 POLY\_3: c-st p q gas  
 ... the command in full is CHANGE\_STATUS  
 Status: /ENTERED/: ENTERED  
 Start value, number of moles /0/: 0  
 POLY\_3:  
 POLY\_3:  
 POLY\_3: s-c t=1473 p=1e5 n=1 x(s)=.33  
 ... the command in full is SET\_CONDITION  
 POLY\_3: c-e  
 ... the command in full is COMPUTE\_EQUILIBRIUM  
 Using global minimization procedure  

Calculated	1978 grid points in	0 s
Found the set of lowest grid points in		0 s
Calculated POLY solution	1 s, total time	1 s

```

POLY_3: l-e
... the command in full is LIST_EQUILIBRIUM
OUTPUT TO SCREEN OR FILE /SCREEN/:
Options /VWCS/: VWCS
Output from POLY-3, equilibrium =      1, label A0 , database: User dat

Conditions:
T=1473, P=1E5, N=1, X(S)=0.33
DEGREES OF FREEDOM 0

Temperature 1473.00 K ( 1199.85 C), Pressure 1.000000E+05
Number of moles of components 1.00000E+00, Mass in grams 5.31576E+01
Total Gibbs energy -1.24169E+05, Enthalpy 1.52783E+04, Volume 0.00000E+00

Component      Moles      W-Fraction  Activity  Potential  Ref.stat
CU              6.7000E-01  8.0094E-01  8.2231E-04 -8.6997E+04 SER
S              3.3000E-01  1.9906E-01  8.3318E-08 -1.9964E+05 SER

QUASI              Status ENTERED      Driving force 0.0000E+00
Moles 1.0000E+00, Mass 5.3158E+01, Volume fraction 0.0000E+00 Mass fractions:
CU 8.00936E-01 S 1.99064E-01
POLY_3:Hit RETURN to continue
POLY_3: s-r-s s gas
... the command in full is SET_REFERENCE_STATE
Temperature /*/: *
Pressure /1E5/: 1E5
POLY_3: sh acr(s)
... the command in full is SHOW_VALUE
ACR(S)=2.1652884E-3
POLY_3:Hit RETURN to continue
POLY_3: s-a-v 1 x(s)
... the command in full is SET_AXIS_VARIABLE
Min value /0/: .3
Max value /1/: .4
Increment /.0025/: .0025
POLY_3: save tcex49 y
... the command in full is SAVE_WORKSPACES
POLY_3: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 0.330000
...OK

Phase Region from 0.330000 for:
QUASI
Global test at 3.50000E-01 .... OK
Global check of adding phase at 3.61133E-01
Calculated 15 equilibria

Phase Region from 0.361133 for:
GAS
QUASI
Global test at 3.80000E-01 .... OK
Terminating at 0.400000
Calculated 19 equilibria

Phase Region from 0.330000 for:
QUASI
Global test at 3.10000E-01 .. Creating a new composition set QUASI#2
Backtracking to find phase change for QUASI#2
Global test at 3.27500E-01 .... OK
Global test at 3.22500E-01 .... OK
Global test at 3.17500E-01 .... OK
Global test at 3.12500E-01 .... OK
Global check of adding phase at 3.11581E-01
Calculated 11 equilibria

Phase Region from 0.311581 for:
QUASI
QUASI#2
Terminating at 0.300000
Calculated 8 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex49\tcex
49.POLY3
POLY_3: po
... the command in full is POST

POLY-3 POSTPROCESSOR VERSION 3.2

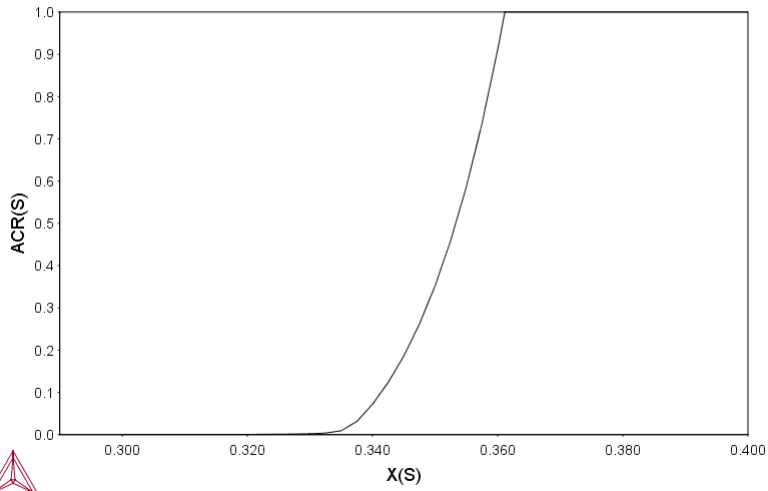
POST: s-d-a x x(s)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y acr(s)
... the command in full is SET_DIAGRAM_AXIS
POST: set-title example 49a
POST: plot
... the command in full is PLOT_DIAGRAM

```



### example 49a

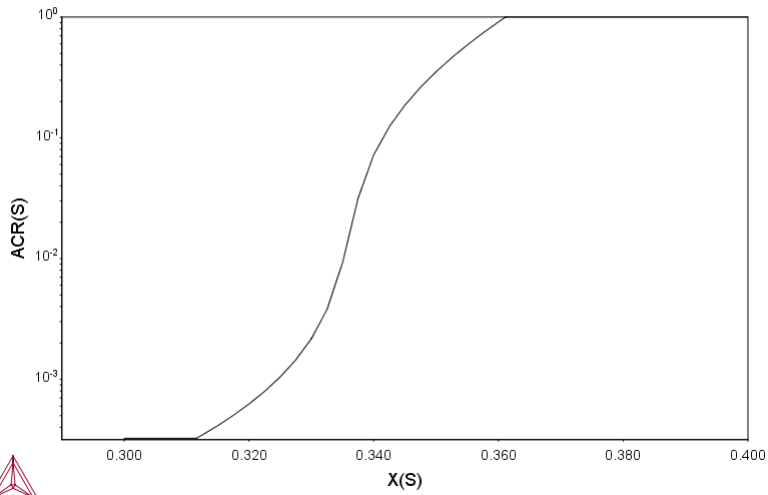
2016.05.16.14.50.59  
User data 2016.05.16: CU, S  
T=1473, P=1E5, N=1



POST:  
POST:Hit RETURN to continue  
POST: s-a-ty y log  
... the command in full is SET\_AXIS\_TYPE  
POST: set-title example 49b  
POST:  
POST: plot  
... the command in full is PLOT DIAGRAM

### example 49b

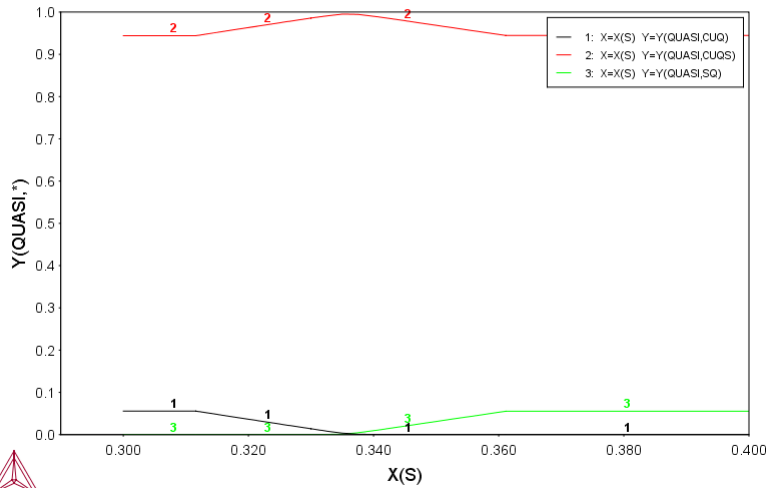
2016.05.16.14.50.59  
User data 2016.05.16: CU, S  
T=1473, P=1E5, N=1



POST:  
POST:Hit RETURN to continue  
POST: s-d-a y y(quasi,\*)  
... the command in full is SET\_DIAGRAM\_AXIS  
COLUMN NUMBER /\*/:  
POST:  
POST: s-a-ty y lin  
... the command in full is SET\_AXIS\_TYPE  
POST: s-lab d  
... the command in full is SET\_LABEL\_CURVE\_OPTION  
POST: set-title example 49c  
POST:  
POST: plot  
... the command in full is PLOT\_DIAGRAM

# example 49c

2016.05.16.14.50.59  
User data 2016.05.16: CU, S  
T=1473, P=1E5, N=1



```
POST:
POST:
POST:@?
POST: back
POLY_3: read tcex49
... the command in full is READ_WORKSPACES
POLY_3:
POLY_3:
POLY_3: s-c t=1573
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      1978 grid points in      0 s
Found the set of lowest grid points in      0 s
Calculated POLY solution      0 s, total time      0 s
POLY_3: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value  0.330000
...OK

Phase Region from  0.330000      for:
  QUASI
Global test at  3.50000E-01 .... OK
Global check of adding phase at  3.56605E-01
Calculated      13 equilibria

Phase Region from  0.356605      for:
  GAS
  QUASI
Global test at  3.75000E-01 .... OK
Global test at  4.00000E-01 .... OK
Terminating at  0.400000
Calculated      21 equilibria

Phase Region from  0.330000      for:
  QUASI
Global test at  3.10000E-01 .... OK
Terminating at  0.300000
Calculated      15 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex49\tcex
49.POLY3
POLY_3:
POLY_3: read tcex49
... the command in full is READ_WORKSPACES
POLY_3:
POLY_3:
POLY_3: s-c t=1673
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      1978 grid points in      1 s
Found the set of lowest grid points in      0 s
Calculated POLY solution      0 s, total time      1 s
POLY_3: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value  0.330000
...OK

Phase Region from  0.330000      for:
  QUASI
Global test at  3.50000E-01 .... OK
Global check of adding phase at  3.52789E-01
Calculated      12 equilibria

Phase Region from  0.352789      for:
  GAS
  QUASI
Global test at  3.72500E-01 .... OK
Global test at  3.97500E-01 .... OK
Terminating at  0.400000
Calculated      22 equilibria

Phase Region from  0.330000      for:
  QUASI
Global test at  3.10000E-01 .... OK
Terminating at  0.300000
Calculated      15 equilibria
```

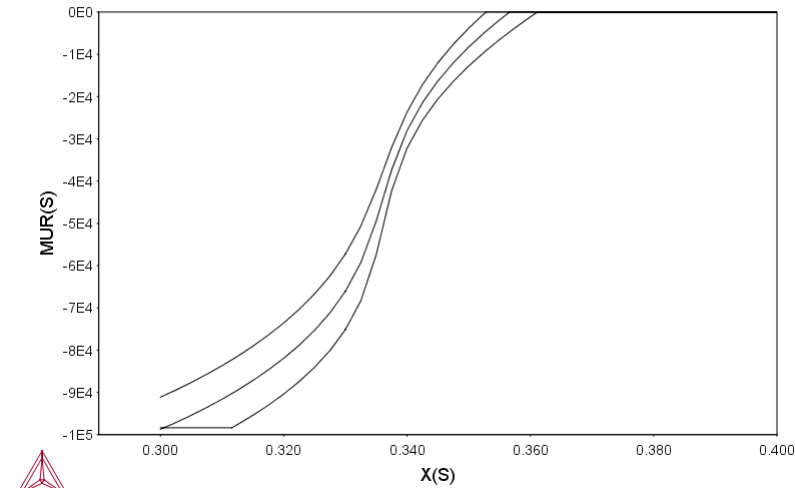
\*\*\* Buffer saved on file:  
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex49.POLY3  
POLY\_3:  
POLY\_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

POST: s-d-a y mur(s)  
... the command in full is SET\_DIAGRAM\_AXIS  
POST: s-d-a x x(s)  
... the command in full is SET\_DIAGRAM\_AXIS  
POST: set-title example 49d  
POST:  
POST: plot  
... the command in full is PLOT DIAGRAM

example 49d

2016.05.16.14.51.02  
User data 2016.05.16: CU, S  
T=1673, P=1E5, N=1.



POST:  
POST: set-inter  
... the command in full is SET\_INTERACTIVE\_MODE  
POST:

## tcex50

**About** Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software (build 9533) running on WinNT 64-bit wordlength  
Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118  
License library version: 8.5.1.0017  
Linked: Mon May 16 09:31:44 2016

**SYS:**SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex50\tcex50.TCM" set-echo

**SYS:** @@

**SYS:** @@ Quasichemical Model via TDB

**SYS:** @@

**SYS:** @@ Calculation of Fig 3+4 in Kongoli et al

**SYS:** @@ Metall. Mater. Trans. B, 29B(1998)591.

**SYS:** @@ Fe-S

**SYS:**

**SYS:** set-log ex50,,,

**SYS:** go da

... the command in full is GOTO\_MODULE

THERMODYNAMIC DATABASE module

Current database: Steels/Fe-Alloys v8.0

VA DEFINED

L12 FCC B2\_BCC B2\_VACANCY

HIGH\_SIGMA DICTRA\_FCC\_A1 REJECTED

**TDB\_TCFE8:** sw user tcex50

... the command in full is SWITCH\_DATABASE

Current database: User defined Database

This database does not support the DATABASE\_INFORMATION command

**TDB\_USER:** d-sys fe s

... the command in full is DEFINE\_SYSTEM

FE S DEFINED

**TDB\_USER:** get

... the command in full is GET\_DATA

ELEMENTS .....

SPECIES .....

PHASES .....

... the command in full is AMEND\_PHASE\_DESCRIPTION

... the command in full is AMEND\_PHASE\_DESCRIPTION

PARAMETERS ...

FUNCTIONS ....

List of references for assessed data

'A T Dinsdale, SGTE lattice stabilities, Calphad 1991'

'Kongoli, Dessureault and Pelton, Met Trans B, 29B (1998) p 591-601'

AFTER ...

-OK-

**TDB\_USER:** go p-3

... the command in full is GOTO\_MODULE

POLY version 3.32

**POLY\_3:** c-st p \*=sus

... the command in full is CHANGE\_STATUS

**POLY\_3:** c-st p quasi=ent 1

... the command in full is CHANGE\_STATUS

**POLY\_3:** s-r-s s quasi \* 1E5

... the command in full is SET\_REFERENCE\_STATE

**POLY\_3:** enter fun lng=log(acr(s)/x(s));

... the command in full is ENTER\_SYMBOL

**POLY\_3:** s-c t=1573 p=1e5 n=1 x(s)=.35

... the command in full is SET\_CONDITION

**POLY\_3:** c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Using global minimization procedure

Calculated 1977 grid points in 1 s

Found the set of lowest grid points in 0 s

Calculated POLY solution 0 s, total time 1 s

**POLY\_3:** s-a-v 1 x(s) 0 .6,,,

... the command in full is SET\_AXIS\_VARIABLE

**POLY\_3:**

**POLY\_3:** s-c t=1473

... the command in full is SET\_CONDITION

**POLY\_3:** c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Using global minimization procedure

Calculated 1977 grid points in 0 s

Found the set of lowest grid points in 0 s

Calculated POLY solution 0 s, total time 0 s

**POLY\_3:** add 1

... the command in full is ADD\_INITIAL\_EQUILIBRIUM

**POLY\_3:** s-c t=1573

... the command in full is SET\_CONDITION

**POLY\_3:** c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Using global minimization procedure

Calculated 1977 grid points in 1 s

Found the set of lowest grid points in 0 s

Calculated POLY solution 0 s, total time 1 s

**POLY\_3:** add 1

... the command in full is ADD\_INITIAL\_EQUILIBRIUM

**POLY\_3:** s-c t=1673

... the command in full is SET\_CONDITION

**POLY\_3:** c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Using global minimization procedure

Calculated 1977 grid points in 0 s

Found the set of lowest grid points in 0 s

Calculated POLY solution 0 s, total time 0 s

**POLY\_3:** add 1

... the command in full is ADD\_INITIAL\_EQUILIBRIUM

**POLY\_3:** s-c t=1773

... the command in full is SET\_CONDITION

**POLY\_3:** c-e

... the command in full is COMPUTE\_EQUILIBRIUM

Using global minimization procedure

Calculated 1977 grid points in 1 s

Found the set of lowest grid points in 0 s

Calculated POLY solution 0 s, total time 1 s

```

POLY_3: add 1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: s-c t=1873
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      1977 grid points in          0 s
Found the set of lowest grid points in        0 s
Calculated POLY solution      0 s, total time  0 s
POLY_3: add 1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: save tcex50 y
... the command in full is SAVE_WORKSPACES
POLY_3: step normal
... the command in full is STEP_WITH_OPTIONS
...OK
...OK
...OK
...OK
...OK

Phase Region from  0.350000      for:
  QUASI
Global test at  4.70000E-01 .... OK
Terminating at   0.600000
Calculated      20 equilibria

Phase Region from  0.350000      for:
  QUASI
Global test at  2.30000E-01 .. Creating a new composition set QUASI#2
Backtracking to find phase change for QUASI#2
Global test at  3.35000E-01 .... OK
Global test at  3.05000E-01 .... OK
Global test at  2.75000E-01 .... OK
Global test at  2.57000E-01 .... OK
Global check of adding phase at  2.55243E-01
Calculated      11 equilibria

Phase Region from  0.255243      for:
  QUASI
  QUASI#2
Global test at  1.46000E-01 .... OK
Global check of removing phase at  1.39331E-01
Calculated      11 equilibria

Phase Region from  0.139331      for:
  QUASI#2
Global test at  2.60000E-02 .... OK
Backtracking to find phase change for QUASI#1
Global test at  1.31000E-01 .... OK
Global test at  1.01000E-01 .... OK
Global test at  7.10000E-02 .... OK
Global test at  4.10000E-02 .... OK
Global test at  1.10000E-02 .... OK
Backtracking to find phase change for QUASI#1
Global check of adding phase at  5.03828E-02
Calculated      11 equilibria

Phase Region from  0.503828E-01 for:
  QUASI
  QUASI#2
Global check of removing phase at  5.03830E-02
Calculated       3 equilibria

Phase Region from  0.503830E-01 for:
  QUASI#2
Terminating at   0.127672E-10
Calculated       7 equilibria

Phase Region from  0.350000      for:
  QUASI
Global test at  4.70000E-01 .... OK
Terminating at   0.600000
Calculated      20 equilibria

Phase Region from  0.350000      for:
  QUASI
Global test at  2.30000E-01 .... OK
Global test at  8.00000E-02 .... OK
Terminating at   0.125999E-10
Calculated      27 equilibria

Phase Region from  0.350000      for:
  QUASI
Global test at  4.70000E-01 .... OK
Terminating at   0.600000
Calculated      20 equilibria

Phase Region from  0.350000      for:
  QUASI
Global test at  2.30000E-01 .... OK
Global test at  8.00000E-02 .... OK
Terminating at   0.124527E-10
Calculated      27 equilibria

Phase Region from  0.350000      for:
  QUASI
Global test at  4.70000E-01 .... OK
Terminating at   0.600000
Calculated      20 equilibria

Phase Region from  0.350000      for:
  QUASI
Global test at  2.30000E-01 .... OK
Global test at  8.00000E-02 .... OK
Terminating at   0.123222E-10
Calculated      27 equilibria

Phase Region from  0.350000      for:
  QUASI
Global test at  4.70000E-01 .... OK
Terminating at   0.600000
Calculated      20 equilibria

Phase Region from  0.350000      for:
  QUASI
Global test at  4.70000E-01 .... OK
Terminating at   0.600000
Calculated      20 equilibria

```

```

QUASI
Global test at 2.30000E-01 .... OK
Global test at 8.00000E-02 .... OK
Terminating at 0.122058E-10
Calculated 27 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex50\tcex
50.POLY3
POLY_3: post

```

POLY-3 POSTPROCESSOR VERSION 3.2

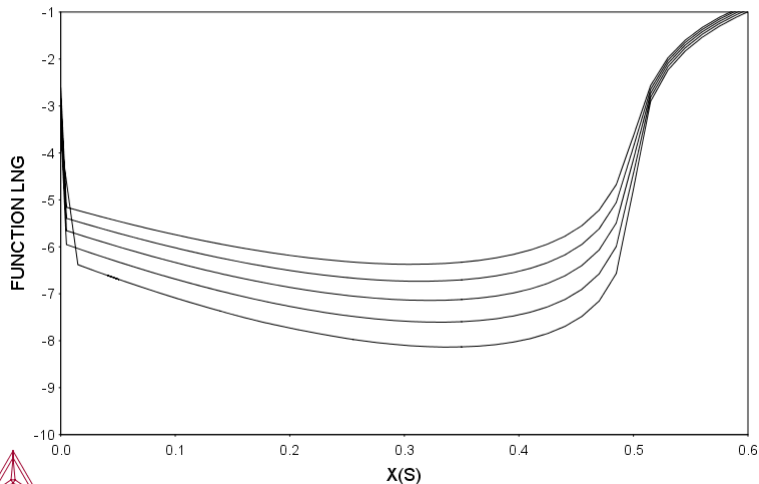
```

POST: s-d-a x x(s)
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y lng
... the command in full is SET_DIAGRAM_AXIS
POST: s-s y n -10 -1
... the command in full is SET_SCALING_STATUS
POST: set-title log(gamma_S) in Fe-S liquid
POST: plot
... the command in full is PLOT DIAGRAM

```

**log(gamma\_S) in Fe-S liquid**

2016.05.16.14.53.20  
 USER: FE,S  
 T=1873, P=1E5, N=1.



```

POST:
POST:Hit RETURN to continue
POST: back
POLY_3: read tcex50
... the command in full is READ_WORKSPACES
POLY_3: rei
... the command in full is REINITIATE_MODULE
POLY_3: c-st p *=sus
... the command in full is CHANGE_STATUS
POLY_3: c-st p quasi=ent 1
... the command in full is CHANGE_STATUS
POLY_3: s-r-s s quasi * 1E5
... the command in full is SET_REFERENCE_STATE
POLY_3: enter fun lng=log(acr(s)/x(s));
... the command in full is ENTER SYMBOL
POLY_3: s-c t=1773 p=1e5 n=1 x(s)=.1
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 1977 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY_3: save tcex50 y
... the command in full is SAVE_WORKSPACES

```

This file contains results from a previous STEP or MAP command.  
 The SAVE command will save the current status of the program but destroy  
 the results from the previous STEP or MAP commands.

```

POLY_3: s-a-v 1 x(s) 0 .14 ,,,
... the command in full is SET_AXIS_VARIABLE
POLY_3: add 1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: s-c t=1823
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 1977 grid points in 1 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 1 s
POLY_3: add 1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: s-c t=1873
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 1977 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 1 s, total time 1 s
POLY_3: add 1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: s-c t=1923
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 1977 grid points in 0 s

```

```

Found the set of lowest grid points in          0 s
Calculated POLY solution          0 s, total time 0 s
POLY_3: add 1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: s-c t=1973
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated          1977 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution          1 s, total time 1 s
POLY_3: add 1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: s-c t=2023
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated          1977 grid points in          0 s
Found the set of lowest grid points in          0 s
Calculated POLY solution          0 s, total time 0 s
POLY_3: add 1
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: step normal
... the command in full is STEP_WITH_OPTIONS
...OK
...OK
...OK
...OK
...OK
...OK
...OK

Phase Region from 0.100000E+00 for:
  QUASI
Global test at 1.28000E-01 .... OK
Terminating at 0.140000
Calculated 15 equilibria

Phase Region from 0.100000E+00 for:
  QUASI
Global test at 7.20000E-02 .... OK
Global test at 3.70000E-02 .... OK
Global test at 2.00000E-03 .... OK
Terminating at 0.123099E-10
Calculated 32 equilibria

Phase Region from 0.100000E+00 for:
  QUASI
Global test at 1.28000E-01 .... OK
Terminating at 0.140000
Calculated 15 equilibria

Phase Region from 0.100000E+00 for:
  QUASI
Global test at 7.20000E-02 .... OK
Global test at 3.70000E-02 .... OK
Global test at 2.00000E-03 .... OK
Terminating at 0.122501E-10
Calculated 32 equilibria

Phase Region from 0.100000E+00 for:
  QUASI
Global test at 1.28000E-01 .... OK
Terminating at 0.140000
Calculated 15 equilibria

Phase Region from 0.100000E+00 for:
  QUASI
Global test at 7.20000E-02 .... OK
Global test at 3.70000E-02 .... OK
Global test at 2.00000E-03 .... OK
Terminating at 0.121935E-10
Calculated 32 equilibria

Phase Region from 0.100000E+00 for:
  QUASI
Global test at 1.28000E-01 .... OK
Terminating at 0.140000
Calculated 15 equilibria

Phase Region from 0.100000E+00 for:
  QUASI
Global test at 7.20000E-02 .... OK
Global test at 3.70000E-02 .... OK
Global test at 2.00000E-03 .... OK
Terminating at 0.121398E-10
Calculated 32 equilibria

Phase Region from 0.100000E+00 for:
  QUASI
Global test at 1.28000E-01 .... OK
Terminating at 0.140000
Calculated 15 equilibria

Phase Region from 0.100000E+00 for:
  QUASI
Global test at 7.20000E-02 .... OK
Global test at 3.70000E-02 .... OK
Global test at 2.00000E-03 .... OK
Terminating at 0.120889E-10
Calculated 32 equilibria

Phase Region from 0.100000E+00 for:
  QUASI
Global test at 1.28000E-01 .... OK
Terminating at 0.140000
Calculated 15 equilibria

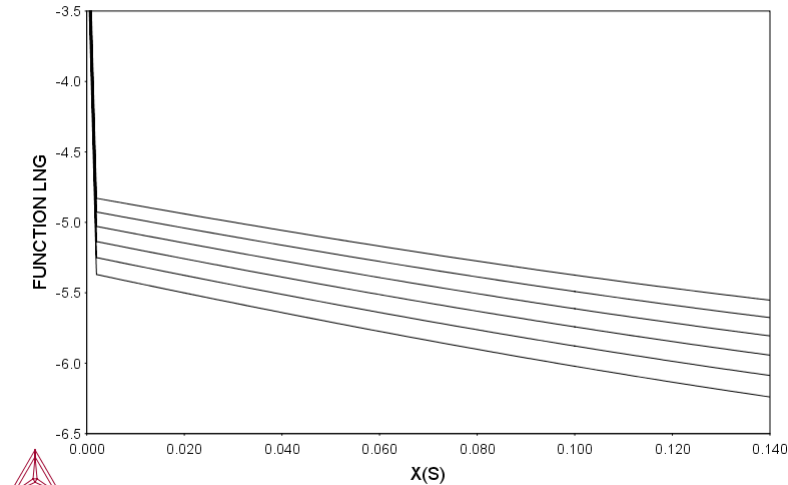
Phase Region from 0.100000E+00 for:
  QUASI
Global test at 7.20000E-02 .... OK
Global test at 3.70000E-02 .... OK
Global test at 2.00000E-03 .... OK
Terminating at 0.120406E-10

```

Calculated 32 equilibria  
 \*\*\* Buffer saved on file:  
 c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex50\tcex50.POLY3  
 POLY\_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

POST: s-d-a x x(s)  
 ... the command in full is SET\_DIAGRAM\_AXIS  
 POST: s-d-a y lng  
 ... the command in full is SET\_DIAGRAM\_AXIS  
 POST: s-s x n 0 .14  
 ... the command in full is SET\_SCALING\_STATUS  
 POST: s-s y n -6.5 -3.5  
 ... the command in full is SET\_SCALING\_STATUS  
 POST: set-title log(gamma\_S)in Fe-S liquid  
 POST:  
 POST: plot  
 ... the command in full is PLOT DIAGRAM  
 log(gamma\_S)in Fe-S liquid  
 2016.05.16.14.53.48  
 USER: FE, S  
 T=2023, P=1E5, N=1.



POST:  
 POST:Hit RETURN to continue  
 POST: back  
 POLY\_3: read tcex50  
 ... the command in full is READ\_WORKSPACES  
 POLY\_3:  
 POLY\_3: rei  
 ... the command in full is REINITIATE\_MODULE  
 POLY\_3: s-c x(s)=.01 t=1900 n=1 p=1e5  
 ... the command in full is SET\_CONDITION  
 POLY\_3: c-e  
 ... the command in full is COMPUTE\_EQUILIBRIUM  
 Using global minimization procedure  
 Calculated 1981 grid points in 0 s  
 Found the set of lowest grid points in 0 s  
 Calculated POLY solution 1 s, total time 1 s  
 POLY\_3: l-e,,,,,  
 ... the command in full is LIST\_EQUILIBRIUM  
 Output from POLY-3, equilibrium = 1, label A0 , database: USER  
 Conditions:  
 X(S)=1E-2, T=1900, N=1, P=1E5  
 DEGREES OF FREEDOM 0  
 Temperature 1900.00 K ( 1626.85 C), Pressure 1.000000E+05  
 Number of moles of components 1.00000E+00, Mass in grams 5.56092E+01  
 Total Gibbs energy -1.19028E+05, Enthalpy 7.56841E+04, Volume 0.00000E+00  

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
FE	9.9000E-01	9.9423E-01	5.9397E-04	-1.1736E+05	SER
S	1.0000E-02	5.7663E-03	5.9092E-05	-1.5381E+05	QUASI

 QUASI Status ENTERED Driving force 0.0000E+00  
 Moles 1.0000E+00, Mass 5.5609E+01, Volume fraction 0.0000E+00 Mass fractions:  
 FE 9.94234E-01 S 5.76631E-03  
 POLY\_3:Hit RETURN to continue  
 POLY\_3: add -2  
 ... the command in full is ADD\_INITIAL\_EQUILIBRIUM  
 POLY\_3: s-c t=1200  
 ... the command in full is SET\_CONDITION  
 POLY\_3: c-e  
 ... the command in full is COMPUTE\_EQUILIBRIUM  
 Using global minimization procedure  
 Calculated 1981 grid points in 0 s  
 Found the set of lowest grid points in 0 s  
 Calculated POLY solution 0 s, total time 0 s  
 POLY\_3: add 1  
 ... the command in full is ADD\_INITIAL\_EQUILIBRIUM  
 POLY\_3: s-a-v 1 x(s) 0 .5 0.01  
 ... the command in full is SET\_AXIS\_VARIABLE  
 POLY\_3: s-a-v 2 t 1000 2000 10  
 ... the command in full is SET\_AXIS\_VARIABLE  
 POLY\_3: save tcex50 y  
 ... the command in full is SAVE\_WORKSPACES  
 This file contains results from a previous STEP or MAP command.  
 The SAVE command will save the current status of the program but destroy  
 the results from the previous STEP or MAP commands.  
 POLY\_3: map  
 Version S mapping is selected



Organizing start points

Using ADDED start equilibria

```
Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4

Phase region boundary 1 at: 5.000E-03 1.792E+03
** BCC_A2
QUASI
Calculated 15 equilibria

Phase region boundary 2 at: 5.000E-03 1.792E+03
** BCC_A2
QUASI
Calculated. 21 equilibria

Phase region boundary 3 at: 6.305E-02 1.667E+03
** BCC_A2
** FCC_A1
QUASI

Phase region boundary 4 at: 6.305E-02 1.667E+03
** FCC_A1
QUASI
Calculated. 162 equilibria

Phase region boundary 5 at: 2.256E-01 1.185E+03
** BCC_A2
** FCC_A1
QUASI

Phase region boundary 6 at: 2.256E-01 1.185E+03
** BCC_A2
QUASI
Calculated.. 20 equilibria
Terminating at axis limit.

Phase region boundary 7 at: 0.000E+00 1.185E+03
** BCC_A2
FCC_A1

Phase region boundary 8 at: 0.000E+00 1.667E+03
BCC_A2
** FCC_A1

Phase region boundary 9 at: 6.305E-02 1.667E+03
** BCC_A2
QUASI
Calculated 65 equilibria

Phase region boundary 10 at: 2.243E-01 1.200E+03
** FCC_A1
QUASI
Calculated. 3 equilibria
Terminating at known equilibrium

Phase region boundary 11 at: 2.243E-01 1.200E+03
** FCC_A1
QUASI
Calculated. 260 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex50\tcex
50.POLY3
CPU time for mapping 8 seconds
POLY_3: po
... the command in full is POST

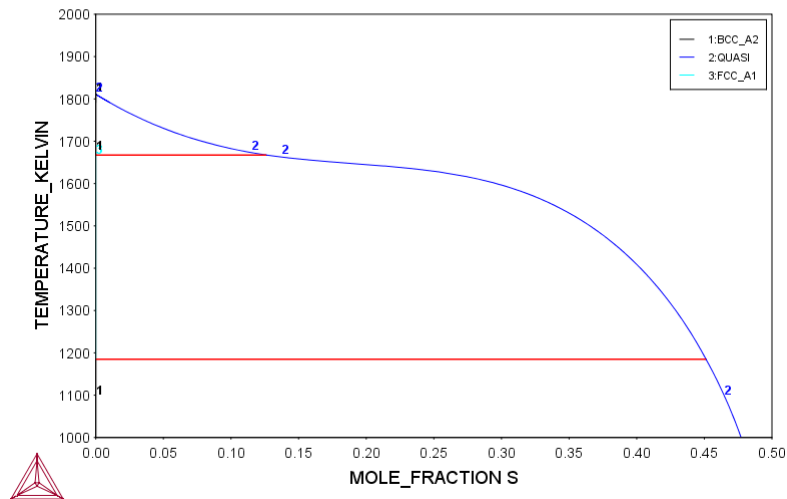
POLY-3 POSTPROCESSOR VERSION 3.2
```

Setting automatic diagram axes

```
POST: set-title Fe-S fcc/liq and bcc/liq
POST: s-l d
... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
... the command in full is PLOT DIAGRAM
```

Fe-S fcc/liq and bcc/liq

2016.05.16 14:54:09  
USER: FE, S  
N=1, P=1E5



```
POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:
```

tcex51

#### SYS>About

Thermo-Calc / DICTRA is software package for calculation of phase diagrams, simulation of phase transformation kinetics and much more.

Copyright Foundation for Computational Thermodynamics,  
Stockholm, Sweden

Software (build 9533) running on WinNT 64-bit wordlength  
Compiler: Intel(R) Visual Fortran Composer Version 13.1.0.149 Build 20130118  
License library version: 8.5.1.0017  
Linked: Mon May 16 09:31:44 2016

SYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex51\tcex51.TCM"SYS: set-echo

SYS: @@

SYS: @@

SYS: @@ Calculation of molar volume, thermal expansivity and density.

SYS: @@

SYS:

SYS: set-log ex51,,

SYS:

SYS: go data

... the command in full is GOTO\_MODULE  
THERMODYNAMIC DATABASE module  
Current database: Steels/Fe-Alloys v8.0

VA DEFINED  
L12\_FCC B2\_BCC B2\_VACANCY  
HIGH\_SIGMA DICTRA\_FCC\_A1 REJECTED

TDB\_TCFE8: sw tofe7

... the command in full is SWITCH\_DATABASE  
Current database: Steels/Fe-Alloys v7.0

VA DEFINED  
L12\_FCC B2\_BCC B2\_VACANCY  
HIGH\_SIGMA DICTRA\_FCC\_A1 REJECTED

TDB\_TCFE7:

TDB\_TCFE7: @@ volume of a unary system

TDB\_TCFE7: d-sys fe

... the command in full is DEFINE\_SYSTEM  
FE DEFINED

TDB\_TCFE7: rej-ph \* all

... the command in full is REJECT

LIQUID:L BCC\_A2 FCC\_A1  
HCP\_A3 A1\_KAPPA KAPPA  
LAVES\_PHASE\_C14 REJECTED

TDB\_TCFE7: rest-ph fcc\_a1,bcc\_a2,liquid

... the command in full is RESTORE  
FCC\_A1 BCC\_A2 LIQUID:L  
RESTORED

TDB\_TCFE7: get

... the command in full is GET\_DATA  
REINITIATING GES5 .....  
ELEMENTS .....  
SPECIES .....  
PHASES .....  
... the command in full is AMEND\_PHASE\_DESCRIPTION  
... the command in full is AMEND\_PHASE\_DESCRIPTION  
PARAMETERS ...  
FUNCTIONS ....

List of references for assessed data

'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'  
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;  
Molar volumes'

-OK-

TDB\_TCFE7:

TDB\_TCFE7: go poly

... the command in full is GOTO\_MODULE

POLY version 3.32

POLY\_3: s-c t=400, n=1, p=1e5

... the command in full is SET\_CONDITION

POLY\_3: c-e

... the command in full is COMPUTE\_EQUILIBRIUM  
Using global minimization procedure  
Calculated 3 grid points in 0 s

POLY\_3: s-a-v 1 t 298 2000,,

... the command in full is SET\_AXIS\_VARIABLE

POLY\_3:

POLY\_3: save tcex51 y

... the command in full is SAVE\_WORKSPACES

POLY\_3: step normal

... the command in full is STEP\_WITH\_OPTIONS  
No initial equilibrium, using default  
Step will start from axis value 400.000

...OK

Phase Region from 400.000 for:  
BCC\_A2  
Global test at 4.80000E+02 .... OK  
Global test at 5.80000E+02 .... OK  
Global test at 6.80000E+02 .... OK  
Global test at 7.80000E+02 .... OK  
Global test at 8.80000E+02 .... OK  
Global test at 9.80000E+02 .... OK  
Global test at 1.08000E+03 .... OK  
Global test at 1.18000E+03 .... OK  
Global check of adding phase at 1.18481E+03  
Calculated 81 equilibria

Phase Region from 1184.81 for:  
BCC\_A2  
FCC\_A1  
Calculated 2 equilibria

Phase Region from 1184.81 for:  
FCC\_A1  
Global test at 1.26000E+03 .... OK  
Global test at 1.36000E+03 .... OK

```

Global test at 1.46000E+03 .... OK
Global test at 1.56000E+03 .... OK
Global test at 1.66000E+03 .... OK
Global check of adding phase at 1.66747E+03
Calculated 51 equilibria

Phase Region from 1667.47 for:
  BCC_A2
  FCC_A1
Calculated 2 equilibria

Phase Region from 1667.47 for:
  BCC_A2
Global Test at 1.74000E+03 .... OK
Global check of adding phase at 1.81095E+03
Calculated 18 equilibria

Phase Region from 1810.95 for:
  LIQUID
  BCC_A2
Calculated 2 equilibria

Phase Region from 1810.95 for:
  LIQUID
Global test at 1.89000E+03 .... OK
Global test at 1.99000E+03 .... OK
Terminating at 2000.00
Calculated 22 equilibria

Phase Region from 400.000 for:
  BCC_A2
Global test at 3.20000E+02 .... OK
Terminating at 298.000
Calculated 14 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex51\tcex
51.POLY3
POLY_3: post

```

```

POLY-3 POSTPROCESSOR VERSION 3.2

```

```

Setting automatic diagram axes

```

```

POST: s-d-a x t-k
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y vm
... the command in full is SET_DIAGRAM_AXIS
POST:
POST: set-title example 51a
POST: s-l e
... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
... the command in full is PLOT DIAGRAM

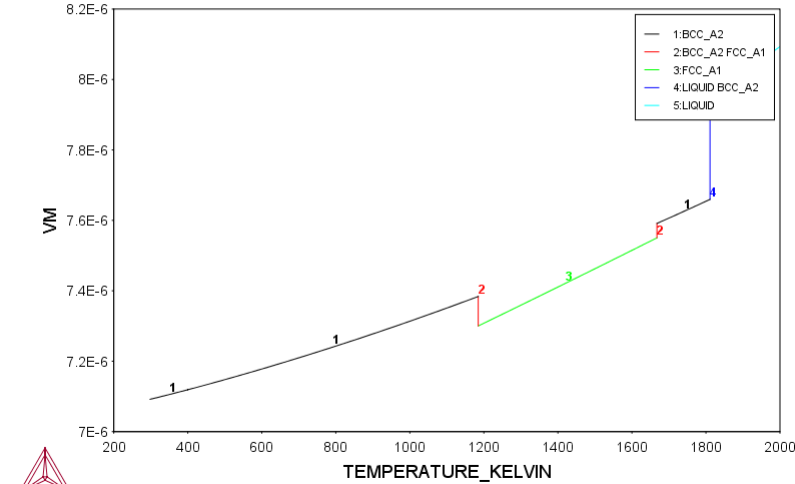
```

example 51a

```

2016.05.16.14.56.30
TCFE7.FE
N=1,P=1E5

```



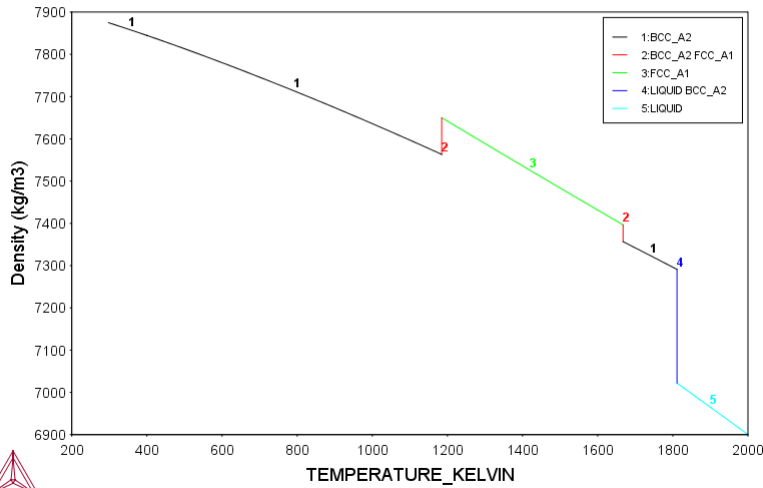
```

POST:
POST:Hit RETURN to continue
POST: @@ define and plot density
POST: ent fun density=b*1e-3/vm;
... the command in full is ENTER_SYMBOL
POST: s-d-a y density
... the command in full is SET_DIAGRAM_AXIS
POST: set-axis-text y n
... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Density (kg/m3)
POST: set-title example 51b
POST:
POST: plot
... the command in full is PLOT_DIAGRAM

```

# example 51b

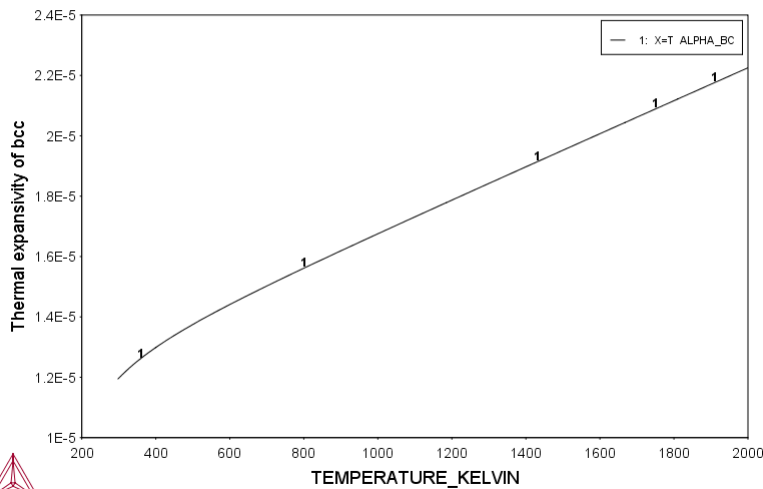
2016.05.16 14:56:30  
TCFE7:FE  
N=1,P=1E5



```
POST:
POST:Hit RETURN to continue
POST: @@ define and plot coefficient of linear
POST: @@ thermal expansion
POST: ent fun alpha_bcc_a2=vm(bcc_a2).t/vm(bcc_a2)/3;
... the command in full is ENTER_SYMBOL
POST: s-d-a y alpha_bcc_a2
... the command in full is SET_DIAGRAM_AXIS
POST: s-l d
... the command in full is SET_LABEL_CURVE_OPTION
POST: set-axis-text y n
... the command in full is SET_AXIS_TEXT_STATUS
AXIS TEXT : Thermal expansivity of bcc
POST: set-title example 51c
POST:
POST: plot
... the command in full is PLOT DIAGRAM
```

# example 51c

2016.05.16 14:56:31  
TCFE7:FE  
N=1,P=1E5



```
POST:
POST:Hit RETURN to continue
POST: back
POLY_3: @@ volume of Fe-C binary system
POLY_3: go da
... the command in full is GOTO_MODULE
TDB_TCFE7: rej sys
... the command in full is REJECT
VA DEFINED
L12 FCC B2_BCC B2_VACANCY
HIGH_SIGMA DICTRA_FCC_A1 REJECTED
REINITIATING GES5 .....
TDB_TCFE7: de-sys fe c
... the command in full is DEFINE_SYSTEM
FE C DEFINED
TDB_TCFE7: rej-ph * all
... the command in full is REJECT
GAS:G LIQUID:L BCC_A2
FCC_A1 HCP_A3 DIAMOND_FCC_A4
GRAPHITE CEMENTITE M23C6
M7C3 M5C2 KSI_CARBIDE
A1_KAPPA KAPPA FE4N_LP1
FE3CN_CHI LAVES_PHASE_C14 REJECTED
TDB_TCFE7: res-ph fcc_a1,bcc_a2,cementite,liquid
... the command in full is RESTORE
FCC_A1 BCC_A2 CEMENTITE
LIQUID:L RESTORED
TDB_TCFE7: get
... the command in full is GET_DATA
REINITIATING GES5 .....
ELEMENTS .....
```

```

SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

'A. Dinsdale, SGTE Data for Pure Elements, Calphad, 15 (1991), 317-425'
'P. Gustafson, Scan. J. Metall., 14 (1985), 259-267; TRITA 0237 (1984); C
-Fe'
'B. Uhrenius (1993-1994), International journal of refractory metals and
hard mater, Vol. 12, pp. 121-127; Molar volumes'
'X.-G. Lu, M. Selleby and B. Sundman, CALPHAD, Vol. 29, 2005, pp. 68-89;
Molar volumes'
'X.-G. Lu, Thermo-Calc Software AB, Sweden, 2006; Molar volumes'
'P. Franke, estimated parameter within SGTE, 2007; Fe-C, Ni-C, Mo-C, C-Mn'
-OK-
TDB_TCFE7:
TDB_TCFE7: go poly
... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3: s-c t=400, n=1, p=1e5
... the command in full is SET_CONDITION
POLY_3: s-c w(c)=.6e-2
... the command in full is SET_CONDITION
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 412 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 0 s, total time 0 s
POLY_3: s-a-v 1 t 298 2000,,
... the command in full is SET_AXIS_VARIABLE
POLY_3:
POLY_3: save tcex51 y
... the command in full is SAVE_WORKSPACES

This file contains results from a previous STEP or MAP command.
The SAVE command will save the current status of the program but destroy
the results from the previous STEP or MAP commands.

POLY_3: step normal
... the command in full is STEP_WITH_OPTIONS
No initial equilibrium, using default
Step will start from axis value 400.000
...OK

Phase Region from 400.000 for:
BCC_A2
CEMENTITE
Global test at 4.80000E+02 .... OK
Global test at 5.80000E+02 .... OK
Global test at 6.80000E+02 .... OK
Global test at 7.80000E+02 .... OK
Global test at 8.80000E+02 .... OK
Global test at 9.80000E+02 .... OK
Global check of adding phase at 9.99783E+02
Calculated 62 equilibria

Phase Region from 999.783 for:
BCC_A2
CEMENTITE
FCC_A1
Calculated 2 equilibria

Phase Region from 999.783 for:
BCC_A2
FCC_A1
Global check of removing phase at 1.02363E+03
Calculated 6 equilibria

Phase Region from 1023.63 for:
FCC_A1
Global test at 1.10000E+03 .... OK
Global test at 1.20000E+03 .... OK
Global test at 1.30000E+03 .... OK
Global test at 1.40000E+03 .... OK
Global test at 1.50000E+03 .... OK
Global test at 1.60000E+03 .... OK
Global check of adding phase at 1.69090E+03
Calculated 70 equilibria

Phase Region from 1690.90 for:
LIQUID
FCC_A1
Global check of removing phase at 1.76294E+03
Calculated 10 equilibria

Phase Region from 1762.94 for:
LIQUID
Global test at 1.84000E+03 .... OK
Global test at 1.94000E+03 .... OK
Terminating at 2000.00
Calculated 27 equilibria

Phase Region from 400.000 for:
BCC_A2
CEMENTITE
Global test at 3.20000E+02 .... OK
Terminating at 298.000
Calculated 14 equilibria
*** Buffer saved on file:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex51\tcex
51.POLY3
POLY_3: post

POLY-3 POSTPROCESSOR VERSION 3.2

Setting automatic diagram axes

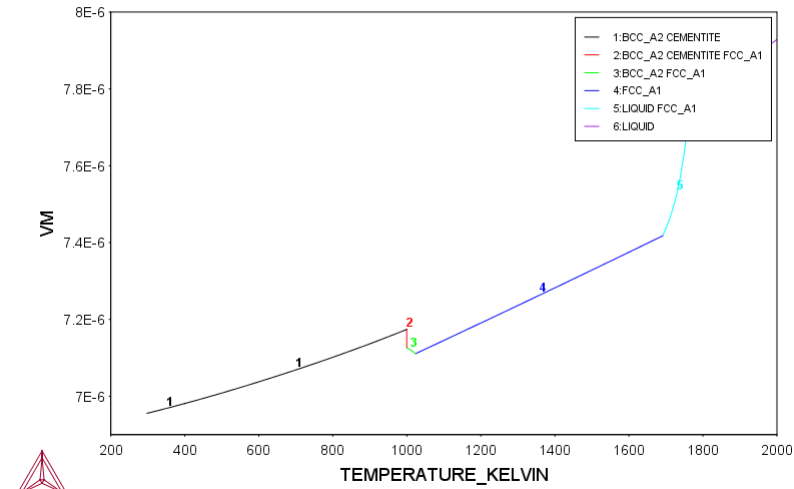
POST: s-d-a x t-k

```

```
... the command in full is SET_DIAGRAM_AXIS
POST: s-d-a y vm
... the command in full is SET_DIAGRAM_AXIS
POST:
POST: set-title example 51d
POST: s-l e
... the command in full is SET_LABEL_CURVE_OPTION
POST: plot
... the command in full is PLOT DIAGRAM
```

example 51d

2016.05.16.14.56.36  
TCFE7: C, FE  
N=1, P=1E5, W(C)=6E-3



```
POST:
POST: set-inter
... the command in full is SET_INTERACTIVE_MODE
POST:
```

AboutSYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex52\tcex52.TCM"SYS: set-echo

SYS: @@  
 SYS: @@ Changing the excess models for interaction  
 SYS: @@ parameters in a solution phase  
 SYS: @@  
 SYS: @@ Example showing how to change the excess models for binary/ternary  
 SYS: @@ interactions in a solution phase, either through direct interactive  
 SYS: @@ amendments of phase descriptions within the GES module, or enforced  
 SYS: @@ by specific type-definitions given in a database file retrieved by  
 SYS: @@ the TDB module.  
 SYS: @@  
 SYS: @@ -----  
 SYS: @@ For Binary Excess Model:  
 SYS: @@ from the default R-K model to Mixed-Excess-Model  
 SYS: @@ (Note the phase has to be a substitutional phase)  
 SYS: @@ -----  
 SYS: @@ For Ternary Extrapolation Model:  
 SYS: @@ from the default R-K-M model to Toop\_Kohler model  
 SYS: @@

SYS: set-log TCX52.LOG

Heading: Example showing how to enter a TOOP binary extrapolation model

SYS: go data  
 ... the command in full is GOTO\_MODULE  
 THERMODYNAMIC DATABASE module  
 Current database: Steels/Fe-Alloys v8.0

VA DEFINED  
 L12\_FCC B2\_BCC B2\_VACANCY  
 HIGH\_SIGMA DICTRA\_FCC\_A1 REJECTED

TDB\_TCFE8: rej sys  
 ... the command in full is REJECT

VA DEFINED  
 L12\_FCC B2\_BCC B2\_VACANCY  
 HIGH\_SIGMA DICTRA\_FCC\_A1 REJECTED  
 REINITIATING GES5 .....

TDB\_TCFE8:  
 TDB\_TCFE8: go gibbs

... the command in full is GOTO\_MODULE  
 GIBBS ENERGY SYSTEM version 5.2

GES:  
 GES: ent-el /- VA A B C  
 ... the command in full is ENTER\_ELEMENT

GES: am\_el\_d /- ELECTRON\_GAS 0.0000E+00 0.0000E+00 0.0000E+00 1  
 ... the command in full is AMEND\_ELEMENT\_DATA  
 GES: am\_el\_d VA VACUUM 0.0000E+00 0.0000E+00 0.0000E+00 1  
 ... the command in full is AMEND\_ELEMENT\_DATA  
 GES: am\_el\_d A UNKNOWN 1.0000E+01 0.0000E+00 0.0000E+00 2  
 ... the command in full is AMEND\_ELEMENT\_DATA  
 GES: am\_el\_d B BETA\_RHOMBO\_B 1.0811E+01 1.2220E+00 5.9000E+00 2  
 ... the command in full is AMEND\_ELEMENT\_DATA  
 GES: am\_el\_d C GRAPHITE 1.2011E+01 1.0540E+00 5.7400E+00 2  
 ... the command in full is AMEND\_ELEMENT\_DATA

GES:  
 GES: ent-phase LIQUID L, 1 A,B,C ; N N  
 ... the command in full is ENTER\_PHASE

GES:  
 GES: ent-param G(LIQUID,A;0) 298.15 0; 6000 N!  
 ... the command in full is ENTER\_PARAMETER  
 G(LIQUID,A;0)-H298(UNKNOWN,A;0)  
 GES: ent-param G(LIQUID,B;0) 298.15 0; 6000 N!  
 ... the command in full is ENTER\_PARAMETER  
 G(LIQUID,B;0)-H298(BETA\_RHOMBO\_B,B;0)  
 GES: ent-param G(LIQUID,C;0) 298.15 0; 6000 N!  
 ... the command in full is ENTER\_PARAMETER  
 G(LIQUID,C;0)-H298(GRAPHITE,C;0)

GES:  
 GES: ent-param L(LIQUID,A,B;0) 298.15 10000; 6000 N  
 ... the command in full is ENTER\_PARAMETER  
 L(LIQUID,A,B;0)  
 GES: ent-param L(LIQUID,A,B;1) 298.15 -10000; 6000 N  
 ... the command in full is ENTER\_PARAMETER  
 L(LIQUID,A,B;1)

GES:  
 GES: list-data ,,  
 Sorry, LIST-DATA disabled for this database

10OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT DATE 2016- 5-16  
 FROM DATABASE: UNKNOWN

ALL DATA IN SI UNITS  
 FUNCTIONS VALID FOR 298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

ELEMENT	STABLE	ELEMENT	REFERENCE	MASS	H298-H0	S298
-1	/-	ELECTRON_GAS		0.0000E+00	0.0000E+00	0.0000E+00
0	VA	VACUUM		0.0000E+00	0.0000E+00	0.0000E+00
1	A	UNKNOWN		1.0000E+01	0.0000E+00	0.0000E+00
2	B	BETA_RHOMBO_B		1.0811E+01	1.2220E+00	5.9000E+00
3	C	GRAPHITE		1.2011E+01	1.0540E+00	5.7400E+00

SPECIES	STOICHIOMETRY
1 A	A
2 B	B
3 C	C
4 VA	VA

Sorry, no data output from this database

LIQUID  
 EXCESS MODEL IS REDLICH-KISTER\_MUGGIANU  
 CONSTITUENTS: A,B,C  
 No data listing for this database

LIST\_OF\_REFERENCES  
 NUMBER SOURCE



```

GES:Hit RETURN to continue
GES:
GES: @@
GES: @@ First Step: Amending the binary excess model:
GES: @@ *****
GES: @@ The default binary excess model is the Redlich-Kister Model for all
GES: @@ the three associated binary interaction pairs (A-B, A-C and B-C)
GES: @@ in the substitutional LIQUID solution phase (without sublattice)
GES: @@ that consists of three elements (A, B and C).
GES: @@
GES: @@ Before changing this default binary excess model for the ternary
GES: @@ LIQUID solution phase, one must have already entered the G
GES: @@ parameters (for standard Gibbs energies of all pure end-members)
GES: @@ and L parameters (for binary R-K excess interaction energies),
GES: @@ as shown here!
GES: @@
GES: @@ In this particular example, we want to change from the default R-K
GES: @@ binary excess model to the Mixed-Excess-Model (with three different
GES: @@ binary excess models, namely Legendre, Polynom and Redlich-Kister
GES: @@ models, applied to the A-B, A-C and B-C binaries, respectively),
GES: @@ as demonstrated below:
GES: @@
GES: @@... For the A-B interaction, the Legendre binary excess model should
GES: @@ be used (rather than the default Redlich-Kister Model), with
GES: @@ the first species (i.e. A) as the independent constituent
GES: @@ and the second species (i.e. B) as the dependent constituent,
GES: @@ while the L parameters for the A-B interaction shall remain
GES: @@ the same as those handled by the R-K model.
GES: @@
GES: amend-phase-description liquid
AMEND WHAT /COMPOSITION_SETS/: ?
You can amend
EXCESS_MODEL
MAGNETIC_ORDERING
DEBYE_HUCKEL
STATUS_BITS
NEW_CONSTITUENT
RENAME_PHASE
COMPOSITION_SETS
GLASS_TRANSITION
DISORDERED_PART
MAJOR_CONSTITUENT
ZRO2_TRANSITION
REMOVE_ADDITIONS
QUASICHEM_IONIC
QUASICHEM_FACT00
QUASICHEM_IRSID
TERNARY_EXTRAPOLAT
HKF_ELECTROSTATIC
DEFAULT_STABLE
SITE_RATIOS
FRACTION_LIMITS
NEVER_DISORDER_PAR
AMEND WHAT /COMPOSITION_SETS/: excess
MODEL NAME /REDLICH-KISTER_MUGGIANU/: ?
REDLICH-KISTER_MUGGIANU
REDLICH-KISTER_KOHLER
FLORY-HUGGINS_POLYMER_MODEL
MIXED-EXCESS-MODELS (R-K default)
HKF
PITZER
CENTRAL_ATOM_MODEL
MODEL NAME /REDLICH-KISTER_MUGGIANU/: mixed
First (the independent) constituent: ?

First (the independent) constituent

Specify the first (the independent) constituent of a certain binary pair
of constituents in the current substitutional solution phase, for which you
wish to change the binary excess model from the default REDLICH-KISTER
model to another model (LEGENDRE or POLYNOM). This sub-option will be
repeatedly prompted (again and again), after having specified the desired
binary Excess model type, for further changes of binary excess model for
other specific binary pair in the current substitutional solution phase.

By simply typing <RETURN> at such a repeated prompt (implying that there
will be no more changes of binary excess model for all other possibly-
remaining binary pairs that shall still use the default REDLICH-KISTER
model), you can finish this MIXED-EXCESS-MODELS option.

First (the independent) constituent: A
Second (the dependent) constituent: B
Excess model type: /LEGENDRE/: ?
Legal choices are: LEGENDRE, POLYNOM or REDLICH-KISTER
Excess model type: /LEGENDRE/: legendre

Any other non-Redlich-Kister binary excess parameters?
First (the independent) constituent: NONE
GES:
GES: list-data ,,
Sorry, LIST-DATA disabled for this database

10OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT      DATE 2016- 5-16
FROM DATABASE:

ALL DATA IN SI UNITS
FUNCTIONS VALID FOR   298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

ELEMENT STABLE ELEMENT REFERENCE  MASS      H298-H0      S298
-1 /-  ELECTRON_GAS                0.0000E+00  0.0000E+00  0.0000E+00
0 VA   VACUUM                      0.0000E+00  0.0000E+00  0.0000E+00
1 A    UNKNOWN                     1.0000E+01  0.0000E+00  0.0000E+00
2 B    BETA_RHOMBO_B               1.0811E+01  1.2220E+00  5.9000E+00
3 C    GRAPHITE                    1.2011E+01  1.0540E+00  5.7400E+00

SPECIES                                STOICHIOMETRY
1 A                                     A
2 B                                     B

```

3 C  
4 VA

C  
VA

Sorry, no data output from this database

LIQUID  
EXCESS MODEL IS MIXED-EXCESS-MODELS (R-K default)  
CONSTITUENTS: A,B,C  
No data listing for this database

LIST\_OF\_REFERENCES  
NUMBER SOURCE

GES:Hit RETURN to continue

GES:

GES: @@... For the A-C interaction, the Polynom binary excess model should  
GES: @@ be used (rather than the default Redlich-Kister Model), with  
GES: @@ the second species (i.e. C) as the independent constituent  
GES: @@ and the first species (i.e. A) as the dependent constituent,  
GES: @@ while the L parameters for the A-C interaction shall remain  
GES: @@ the same as those handled by the R-K model.  
GES: @@

GES: ent-param G(LIQUID,A,C;0) 298.15 10000; 6000 N  
... the command in full is ENTER\_PARAMETER  
G(LIQUID,A,C;0)

GES: ent-param G(LIQUID,A,C;1) 298.15 5000; 6000 N  
... the command in full is ENTER\_PARAMETER  
G(LIQUID,A,C;1)

GES:

GES: amend-phase-des LIQUID excess mixed C A polynom  
... the command in full is AMEND\_PHASE\_DESCRIPTION

Any other non-Redlich-Kister binary excess parameters?

First (the independent) constituent:

GES: list-data ,,  
Sorry, LIST-DATA disabled for this database

10OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT DATE 2016- 5-16  
FROM DATABASE:

ALL DATA IN SI UNITS  
FUNCTIONS VALID FOR 298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

ELEMENT	STABLE	ELEMENT	REFERENCE	MASS	H298-H0	S298
-1	/-	ELECTRON_GAS		0.0000E+00	0.0000E+00	0.0000E+00
0	VA	VACUUM		0.0000E+00	0.0000E+00	0.0000E+00
1	A	UNKNOWN		1.0000E+01	0.0000E+00	0.0000E+00
2	B	BETA_RHOMBO_B		1.0811E+01	1.2220E+00	5.9000E+00
3	C	GRAPHITE		1.2011E+01	1.0540E+00	5.7400E+00

SPECIES	STOICHIOMETRY
1 A	A
2 B	B
3 C	C
4 VA	VA

Sorry, no data output from this database

LIQUID  
EXCESS MODEL IS MIXED-EXCESS-MODELS (R-K default)  
CONSTITUENTS: A,B,C  
No data listing for this database

LIST\_OF\_REFERENCES  
NUMBER SOURCE

GES:Hit RETURN to continue

GES:

GES: @@... For the B-C interaction, the default Redlich-Kister binary  
GES: @@ excess model shall still be used; so we do not need to amend  
GES: @@ anything regarding that.  
GES: @@

GES: ent-param G(LIQUID,B,C;0) 298.15 10000; 6000 N  
... the command in full is ENTER\_PARAMETER  
G(LIQUID,B,C;0)

GES: ent-param G(LIQUID,B,C;1) 298.15 -2000; 6000 N  
... the command in full is ENTER\_PARAMETER  
G(LIQUID,B,C;1)

GES:

GES: list-data ,,  
Sorry, LIST-DATA disable for this database

10OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT DATE 2016- 5-16  
FROM DATABASE:

ALL DATA IN SI UNITS  
FUNCTIONS VALID FOR 298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

ELEMENT	STABLE	ELEMENT	REFERENCE	MASS	H298-H0	S298
-1	/-	ELECTRON_GAS		0.0000E+00	0.0000E+00	0.0000E+00
0	VA	VACUUM		0.0000E+00	0.0000E+00	0.0000E+00
1	A	UNKNOWN		1.0000E+01	0.0000E+00	0.0000E+00
2	B	BETA_RHOMBO_B		1.0811E+01	1.2220E+00	5.9000E+00
3	C	GRAPHITE		1.2011E+01	1.0540E+00	5.7400E+00

SPECIES	STOICHIOMETRY
1 A	A
2 B	B
3 C	C
4 VA	VA

Sorry, no data output from this database

LIQUID  
EXCESS MODEL IS MIXED-EXCESS-MODELS (R-K default)  
CONSTITUENTS: A,B,C  
No data listing for this database

LIST\_OF\_REFERENCES  
NUMBER SOURCE

GES:Hit RETURN to continue

GES:  
GES: @@  
GES: @@Second Step: Amending the ternary extrapolation model:  
GES: @@\*\*\*\*\* =====  
GES: @@The default ternary excess model is the Redlich-Kister Muggianu  
GES: @@ Model (i.e., the MUGGIANU\_RESTOR method for ternary extrapolation  
GES: @@ based on binary parameters) for the associated ternary interaction  
GES: @@ terms; when no ternary L parameter is entered for that, such a  
GES: @@ default Redlich-Kister\_Muggianu Model is thus to be used for  
GES: @@ extrapolation from binary excess energies to ternary interactions  
GES: @@ in the substitutional LIQUID solution phase (without sublattice)  
GES: @@ that consists of three elements (A, B and C).  
GES: @@  
GES: @@However, in this particular example as illustrated in the following,  
GES: @@ we shall change from this default R-K-M ternary excess model to  
GES: @@ the TOOP-KOHLER method for the ternary extrapolation method, with  
GES: @@ the species C as the Toop constituent, while the species A and B  
GES: @@ as the Kohler constituents (entering A and B, or B and A, as the  
GES: @@ basis constituent and first interacting constituent). This will  
GES: @@ implicitly enforce that, during the ternary extrapolation, only  
GES: @@ the A-B binary interaction parameters are utilized in accordance  
GES: @@ with the Kohler ternary extrapolation formula for A-B-C ternary  
GES: @@ interaction, while any other binary interaction parameters  
GES: @@ involving the Toop species C (i.e., of A-C and B-C binaries) are  
GES: @@ used in line with the Toop-Kohler ternary extrapolation formula  
GES: @@ (for the A-C-B and B-C-A ternary interactions). This makes the  
GES: @@ extrapolated ternary excess interaction terms different from  
GES: @@ those handled either by the default MUGGIANU\_RESTOR method  
GES: @@ or by the alternative KOHLER-ALL method.  
GES: @@  
GES: @@Note that only when all the relevant binary excess energies in a  
GES: @@ ternary system are treated by the default Redlich-Kister Model  
GES: @@ (i.e., the Mixed-Excess-Model should have not been used), the  
GES: @@ MUGGIANU\_RESTOR method for ternary extrapolations is equivalent  
GES: @@ to the Redlich-Kister\_Muggianu Model, or the KOHLER-ALL method  
GES: @@ to the Redlich-Kister\_Kohler Model.  
GES: @@

GES: amend\_phase-des LIQUID  
... the command in full is AMEND\_PHASE\_DESCRIPTION

AMEND WHAT /COMPOSITION\_SETS/: ?

You can amend  
EXCESS\_MODEL  
MAGNETIC\_ORDERING  
DEBYE\_HUCKEL  
STATUS\_BITS  
NEW\_CONSTITUENT  
RENAME\_PHASE  
COMPOSITION\_SETS  
GLASS\_TRANSITION  
DISORDERED\_PART  
MAJOR\_CONSTITUENT  
ZRO2\_TRANSITION  
REMOVE\_ADDITIONS  
QUASICHEM\_IONIC  
QUASICHEM\_FACT00  
QUASICHEM\_IRSID  
TERNARY\_EXTRAPOLAT  
HKF\_ELECTROSTATIC  
DEFAULT\_STABLE  
SITE\_RATIOS  
FRACTION\_LIMITS  
NEVER\_DISORDER\_PAR

AMEND WHAT /COMPOSITION\_SETS/: TERN-EXT

Extrapolation method: /TOOP-KOHLER/: ?

Default method is Muggianu, you can use  
TOOP-KOHLER  
KOHLER-ALL  
MUGGIANU\_RESTOR

Extrapolation method: /TOOP-KOHLER/: TOOP-KOHLER

Constituent in sublattice 1: A

First interaction constituent: B

Toop constituent: C

GES:

GES: list-data ,,  
Sorry, LIST-DATA disabled for this database

10OUTPUT FROM GIBBS ENERGY SYSTEM ON PC/WINDOWS NT DATE 2016- 5-16  
FROM DATABASE:

ALL DATA IN SI UNITS  
FUNCTIONS VALID FOR 298.15<T< 6000.00 K UNLESS OTHER LIMITS STATED

ELEMENT	STABLE	ELEMENT	REFERENCE	MASS	H298-H0	S298
-1	/-	ELECTRON_GAS		0.0000E+00	0.0000E+00	0.0000E+00
0	VA	VACUUM		0.0000E+00	0.0000E+00	0.0000E+00
1	A	UNKNOWN		1.0000E+01	0.0000E+00	0.0000E+00
2	B	BETA_RHOMBO_B		1.0811E+01	1.2220E+00	5.9000E+00
3	C	GRAPHITE		1.2011E+01	1.0540E+00	5.7400E+00

SPECIES	STOICHIOMETRY
1 A	A
2 B	B
3 C	C
4 VA	VA

Sorry, no data output from this database

LIQUID  
EXCESS\_MODEL IS MIXED-EXCESS-MODELS (R-K default)  
CONSTITUENTS: A,B,C  
No data listing for this database

LIST\_OF\_REFERENCES  
NUMBER SOURCE

GES:Hit RETURN to continue

```

GES:
GES: @@ Third Step: Performing an equilibrium calculation
GES: @@          using the entered and amended descriptions.
GES: @@ ***** =====
GES: @@
GES: go p-3
    ... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3: s-c t=1500 p=1e5 n=1 x(b)=.2 x(c)=.3
    ... the command in full is SET_CONDITION
POLY_3: c-e
    ... the command in full is COMPUTE_EQUILIBRIUM
    Using global minimization procedure
    Calculated          1977 grid points in          0 s
    Found the set of lowest grid points in          0 s
    Calculated POLY solution          0 s, total time    0 s
POLY_3: l-e , X
    ... the command in full is LIST_EQUILIBRIUM
    Output from POLY-3, equilibrium =          1, label A0 , database:

Conditions:
T=1500, P=1E5, N=1, X(B)=0.2, X(C)=0.3
DEGREES OF FREEDOM 0

Temperature 1500.00 K ( 1226.85 C), Pressure 1.000000E+05
Number of moles of components 1.000000E+00, Mass in grams 1.07655E+01
Total Gibbs energy -1.08432E+04, Enthalpy 1.99843E+03, Volume 0.000000E+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 5.0000E-01 C 3.0000E-01 B 2.0000E-01
POLY_3: sh qf(*)
    ... the command in full is SHOW_VALUE
    QF(LIQUID)=0.52168269
POLY_3: sh gm(*) dgm(*)
    ... the command in full is SHOW_VALUE
    GM(LIQUID)=-10843.162
    DGM(LIQUID)=0
POLY_3:
POLY_3: save TCEX52a.POLY3 y
    ... the command in full is SAVE_WORKSPACES
POLY_3:Hit RETURN to continue
POLY_3:
POLY_3: @@ Fourth Step: Reading the same data from a small database and
POLY_3: @@          Performing the same equilibrium calculation.
POLY_3: @@ ***** =====
POLY_3: @@
POLY_3: go data
    ... the command in full is GOTO_MODULE
TDB_TCFE8: rej sys
    ... the command in full is REJECT
VA DEFINED
L12 FCC          B2_BCC          B2_VACANCY
HIGH_SIGMA      DICTRA_FCC_A1 REJECTED
REINITIATING GES5 .....
TDB_TCFE8:
TDB_TCFE8: sw user TCEX52-TOOP.TDB
    ... the command in full is SWITCH_DATABASE
    Current database: User defined Database
    This database does not support the DATABASE_INFORMATION command

VA          /- DEFINED
TDB_USER: d-sys /all
    ... the command in full is DEFINE_SYSTEM
A          B          C
    DEFINED
TDB_USER: l-sys const
    ... the command in full is LIST_SYSTEM
LIQUID:L :A B C:
TDB_USER: get
    ... the command in full is GET_DATA
ELEMENTS .....
SPECIES .....
PHASES .....
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

'Reference 2'
'Reference 1'
AFTER ...
    ... the command in full is AMEND_PHASE_DESCRIPTION
    ... the command in full is AMEND_PHASE_DESCRIPTION
-OK-
TDB_USER:
TDB_USER:Hit RETURN to continue
TDB_USER: go p-3
    ... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3:
POLY_3: s-c t=1500 p=1e5 n=1 x(b)=.2 x(c)=.3
    ... the command in full is SET_CONDITION
POLY_3: c-e
    ... the command in full is COMPUTE_EQUILIBRIUM
    Using global minimization procedure
    Calculated          1977 grid points in          0 s
    Found the set of lowest grid points in          0 s
    Calculated POLY solution          0 s, total time    0 s
POLY_3: l-e , X
    ... the command in full is LIST_EQUILIBRIUM
    Output from POLY-3, equilibrium =          1, label A0 , database: USER

Conditions:
T=1500, P=1E5, N=1, X(B)=0.2, X(C)=0.3
DEGREES OF FREEDOM 0

```

Temperature 1500.00 K ( 1226.85 C), Pressure 1.000000E+05  
Number of moles of components 1.00000E+00, Mass in grams 1.07655E+01  
Total Gibbs energy -1.08432E+04, Enthalpy 1.99843E+03, Volume 0.00000E+00

Component	Moles	M-Fraction	Activity	Potential	Ref.stat
A	5.0000E-01	5.0000E-01	4.7833E-01	-9.1973E+03	SER
B	2.0000E-01	2.0000E-01	1.9875E-01	-2.0151E+04	SER
C	3.0000E-01	3.0000E-01	5.5332E-01	-7.3811E+03	SER

LIQUID Status ENTERED Driving force 0.0000E+00  
Moles 1.0000E+00, Mass 1.0765E+01, Volume fraction 0.0000E+00 Mole fractions:  
A 5.00000E-01 C 3.00000E-01 B 2.00000E-01

POLY\_3: sh qf(\*)  
... the command in full is SHOW\_VALUE  
QF(LIQUID)=0.52168269  
POLY\_3: sh gm(\*) dgm(\*)  
... the command in full is SHOW\_VALUE  
GM(LIQUID)=-10843.162  
DGM(LIQUID)=0  
POLY\_3:  
POLY\_3: save TCEX52b.POLY3 y  
... the command in full is SAVE\_WORKSPACES  
POLY\_3:  
POLY\_3: @@  
POLY\_3: @@ As you have noticed above, the calculated equilibrium (using the  
POLY\_3: @@ small database) is exactly the same as the first calculation  
POLY\_3: @@ (with data amended in the GES module step-by-step, for the  
POLY\_3: @@ binary/ternary excess models).  
POLY\_3: @@  
POLY\_3:  
POLY\_3: set-inter  
... the command in full is SET\_INTERACTIVE  
POLY\_3:

AboutSYS:SYS:MACRO "c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex53\tcex53.TCM"SYS:SYS:SYS:

SYS:SYS: set-echo  
SYS:

SYS: set-log TCEX53.LOG

Heading: Pourbaix Diagram Calculations through the TDB-GES-POLY-POST routine

SYS: @@  
SYS: @@ TCEX53: Thermo-Calc 4.0 (Console Mode) Standard Example No 53  
SYS: @@ \*\*\*\*\*  
SYS: @@ Copyright: Thermo-Calc Software AB, Stockholm, Sweden  
SYS: @@ Developer: Dr. Pingfang Shi, Thermo-Calc Software AB  
SYS: @@ Date: 2014-05-26 (revision)  
SYS: @@

SYS: @@ Pourbaix Diagram Calculations through the TDB-GES-POLY-POST routine  
SYS: @@ \*\*\*\*\*

SYS: @@ \* Using PAQ2 or PAQS2 database;  
SYS: @@ \* For the Fe-X-H2O-NaCl heterogeneous interaction systems  
SYS: @@ (X = Cr-Ni-Co)

SYS: @@ Note: The PAQ2 (TCS Public Aqueous Solution (SIT) Database, v2.4;  
SYS: @@ using the SIT aqueous solution model) or PAQS2 (TCS Public  
SYS: @@ Aqueous Solution Database, v2.4; using the Complete Revised  
SYS: @@ HKF aqueous solution model) contains an AQUEOUS solution  
SYS: @@ phase and REF\_ELECTRODE phase (as a reference for electron  
SYS: @@ in aqueous electrolyte systems), as well as some data for  
SYS: @@ various solid phases (solution or stoichiometric) and  
SYS: @@ gaseous mixture phase. Therefore, it can be used, via the  
SYS: @@ Single-Database Option in the POURBAIX module or through  
SYS: @@ the normal TDB-GES-PLOY-POST routine, for calculations of  
SYS: @@ the so-called Pourbaix diagrams (i.e., pH-Eh plots) and  
SYS: @@ other types of diagrams in aqueous-bearing multicomponent  
SYS: @@ heterogeneous interaction systems.

SYS: @@ Also Note: The initial bulk composition of Fe-based alloy in this  
SYS: @@ demonstrating calculation is just preliminarily assigned,  
SYS: @@ in which the BCC\_A2 and/or FCC\_A1 solution phase(s) are  
SYS: @@ considered as of primarily interest.  
SYS: @@ For practical calculations, one shall have more precise  
SYS: @@ inputs for the initial bulk compositions of alloys.

SYS: @@ -----  
SYS: @@

SYS: @@ -----  
SYS: @@

SYS: @@ Step 1: Single-Point Calculations for H2O-NaCl system  
SYS: @@ \*\*\*\*\*

SYS: @@ To demonstrate how to define the molality of NaCl  
SYS: @@ in an aqueous-bearing heterogeneous interaction system  
SYS: @@

SYS: @@... Retrieving data from the PAQ2 or PAQS2 database:  
SYS: go data

... the command in full is GOTO\_MODULE  
THERMODYNAMIC DATABASE module  
Current database: Steels/Fe-Alloys v8.0

VA DEFINED  
L12\_FCC B2\_BCC B2\_VACANCY  
HIGH\_SIGMA DICTRA\_FCC\_A1 REJECTED

TDB\_TCFE8: rej sys  
... the command in full is REJECT

VA DEFINED  
L12\_FCC B2\_BCC B2\_VACANCY  
HIGH\_SIGMA DICTRA\_FCC\_A1 REJECTED  
REINITIATING GES5 .....

TDB\_TCFE8: @@ ----- switch on PAQ2 or PAQS2

TDB\_TCFE8: sw PAQ2  
... the command in full is SWITCH\_DATABASE  
Current database: Public Aqueous Soln (SIT) TDB v2.4

H O ZE  
VA DEFINED  
LIQUID:L REJECTED  
GRAPHITE DIAMOND\_A4 FC\_ORTHORHOMBIC  
MONOCLINIC REJECTED  
CBCC\_A12 CUB\_A13 CHI\_A12  
FE4N FECN\_CHI REJECTED  
CEMENTITE M23C6 M7C3  
M5C2 M3C2 KSI\_CARBIDE  
PI REJECTED  
FE3C NI3C CR3C2  
CR7C3 CR23C6 REJECTED  
COCO3 FECO3 NAHCO3  
NA2CO3 NA2CO3\_S2 NICO3  
CRC6O6 REJECTED  
CO3N CRN CR2N  
FE2N NI3N REJECTED  
NANO2 NANO2\_S2 NANO3  
REJECTED  
COCL2 CRCL2 CRCL3  
FECL2 FECL3 NICL2  
REJECTED  
FECLO NACL04 NACL04\_S2  
REJECTED

TDB\_PAQ2: data  
... the command in full is DATABASE\_INFORMATION  
Current database: Public Aqueous Soln (SIT) TDB v2.4

PAQ2  
Thermo-Calc PUBLIC AQUEOUS DATABASE FOR POURBAIX MODULE  
(based on and replacing AQ in TCC/TCW & PAQ in TCC-Demo/TCW-Demo)  
\*\*\*\*\*  
(Version 2.4, Feb. 2008)

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This public aqueous solution database contains aqueous solution species,  
and gaseous mixture species and solid/liquid (pure and solution) phases  
in an 11-element system (Fe-Co-Cr-Na-Ni-C-H-O-N-S-Cl). As a demo version  
of the complete TCAQ2 Aqueous Solution Database, it is specially designed

for uses with the apecial POURBAIX module which allows easy and automatic calculations of the sp-called Pourbaix diagrams (i.e., Eh-pH plots) and many types of property diagrams. It can also be used in normal TCC/TCW calculations for aqueous involved heterogeneous 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 heterogeneous 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, CCCL, 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 potential [MUR(ZE)], while this phase should always be SUSPENDED in all the POLY calculations.

For further information, please contact Dr. Pingfang Shi at TCSAB.

Release History: Version 1.0 initial release (as AQ), 1997  
Version 1.1 with minor improvements (as AQ), 1998  
Version 1.2 with minor improvements (as AQ), 2000  
Version 2.0 with major improvements (as PAQ2.0), 2002  
Version 2.1 with minor improvements (as PAQ2.1), 2003  
Version 2.2 with minor improvements (as PAQ2.2), 2006  
Version 2.3 with minor improvements (as PAQ2.3), 2007  
Version 2.4 with major improvements (as PAQ2.4), 2008

Edited by: Dr. Pingfang Shi (Thermo-Calc Software, 1997-2008).

```
TDB_PAQ2: d-sys H O Na Cl
... the command in full is DEFINE_SYSTEM
NA                                CL    DEFINED
TDB_PAQ2: l-sys const
... the command in full is LIST_SYSTEM
```

```

AQUEOUS:A      :H2O H2 H+1 OH-1 H2O2 HO2-1 O2 O3 CL2 CL-1 CLO2 CLO-1 CLO2-1
CLO3-1 CLO4-1 HCLO HCLO2 NA+1:
> Aqueous Solution: using the SIT Model (from TCAQ2 database)
REF ELECTRODE :ZE:
> Reference Electrode for ZE potential; always SUSPENDED in POLY.
GAS:G         :CL CL2 CL1H1 CL1O1 CL1O2 CL1H1O1 CL2O1 CL1NA1 CL2NA2 CL3NA3 H
H1NA1 H1NA1O1 H1O1 H1O2 H2 H2NA2O2 H2O1 H2O2 NA NA1O1 NA2 NA2O1 NA2O2 O O2
O3:
> Gaseous Mixture, using the ideal gas model
FCC_A1        :NA O:VA:
> This is also the MX (X=C,N) solution phase.
BCC_A2        :NA O:VA:
> This is also the MX3 (X=C,N) solution phase.
HCP_A3        :NA:VA:
> This is also the M2X (X=C,N) solution phase.
HALITE        :NA1CL1:
NAO2          :NA1O2:
NA2O          :NA2O1:
NA2O_S2       :NA2O1:
NA2O_S3       :NA2O1:
NA2O2         :NA2O2:
NA2O2_S2      :NA2O2:
NAOH          :H1NA1O1:
NAOH_S2       :H1NA1O1:
TDB_PAQ2: get
... the command in full is GET_DATA
REINITIATING GES5 .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

'TCS public data set for gaseous mixture in the Fe-Co-Cr-Na-Ni-C-H-O-N-S
-Cl system.'
'TCS public data set for liquid mixture and alloy solutions in the Fe-Co
-Cr-Na-Ni-C-H-O-N-S-Cl system.'
'TCS public data set for stoichiometric solids and liquids in the Fe-Co-Cr
-Na-Ni-C-H-O-N-S-Cl system.'
'TCS Aqueous Solution Database, TCAQ2, v2.0 (2002/2003). Extracted data
only for Fe-Co-Cr-Na-Ni-C-H-O-N-S-Cl bearing aqueous solution species
from TCAQ2 which covers totally 83 elements and contains many more
aqueous solution species.'
-OK-
TDB_PAQ2:Hit RETURN to continue
TDB_PAQ2:
TDB_PAQ2: @@... Defining system-components and their proper reference states:
TDB_PAQ2: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3: d-com H2O H+1 ZE Na Cl
... the command in full is DEFINE_COMPONENTS
POLY_3: s-r-s H2O AQUEOUS * 1e5
... the command in full is SET_REFERENCE_STATE
POLY_3: s-r-s ZE REF_ELE * 1e5
... the command in full is SET_REFERENCE_STATE
POLY_3: l-st c
... the command in full is LIST_STATUS
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS      REF. STATE      T(K)          P(Pa)
VA              ENTERED      SER
H2O             ENTERED      AQUEOUS        *              100000
H+1             ENTERED      SER
ZE              ENTERED      REF ELECTRODE  *              100000
NA              ENTERED      SER
CL              ENTERED      SER
POLY_3:
POLY_3: @@... Defining the equilibrium conditions:
POLY_3: @@ -----
POLY_3: @@ Defining P-T and bulk composition in the interaction system
POLY_3: @@ for the calculations of initial equilibria:
POLY_3: @@
POLY_3: s-c P=1e5 T=298.15 b(H2O)=1000
... the command in full is SET_CONDITION
POLY_3: s-in-am b(Na1Cl1)=5
... the command in full is SET_INPUT_AMOUNTS
POLY_3: s-c n(H+1)=0 n(ZE)=0
... the command in full is SET_CONDITION
POLY_3: l-c
... the command in full is LIST_CONDITIONS
P=1E5, T=298.15, B(H2O)=1000, B(NA)=1.96686, B(CL)=3.03314, N(H+1)=0,
N(ZE)=0
DEGREES OF FREEDOM 0
POLY_3:
POLY_3: @@... Calculating an equilibrium with only AQUEOUS presented:
POLY_3: c-st p *=sus
... the command in full is CHANGE_STATUS
POLY_3: c-st p AQUEOUS=ent 55.8
... the command in full is CHANGE_STATUS
POLY_3: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE          STATUS      DRIVING FORCE      MOLES
AQUEOUS        ENTERED      0.000000E+00      1.785600E+03
SUSPENDED PHASES:
REF ELECTRODE NAOH_S2 NAOH NAO2 NA2O_S3 NA2O_S2 NA2O2_S2 NA2O2 NA2O HCP_A3
HALITE FCC_A1 BCC_A2 GAS
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      17 grid points in      0 s
Found the set of lowest grid points in      0 s
Creating a new composition set AQUEOUS#2
Creating a new composition set AQUEOUS#3
Calculated POLY solution      0 s, total time      0 s

```



```

POLY_3: l-e ,x
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: PAQ2

Conditions:
P=1E5, T=298.15, B(H2O)=1000, B(NA)=1.96686, B(CL)=3.03314, N(H+1)=0,
N(ZE)=0
DEGREES OF FREEDOM 0

Temperature 298.15 K ( 25.00 C), Pressure 1.000000E+05
Number of moles of components 5.56795E+01, Mass in grams 1.00500E+03
Total Gibbs energy -1.70630E+07, Enthalpy -1.59010E+07, Volume 0.00000E+00

Component      Moles      M-Fraction  Activity  Potential  Ref.stat
H2O             5.5508E+01  9.9693E-01  9.9654E-01 -8.5871E+00 AQUEOUS
H+1             -9.7239E-08 -1.7464E-09  1.0405E-07 -3.9858E+04 SER
ZE             8.6043E-08  1.5453E-09  3.4476E+12  7.1565E+04 REF_ELEC
NA             8.5554E-02  1.5365E-03  4.5046E-63 -3.5588E+05 SER
CL             8.5554E-02  1.5365E-03  4.1623E-18 -9.9210E+04 SER

AQUEOUS          Status ENTERED      Driving force 0.0000E+00
Moles 5.5680E+01, Mass 1.0050E+03, Volume fraction 0.0000E+00 Mole fractions:
H2O 9.96927E-01 NA 1.53654E-03 H+1 -1.74641E-09
CL 1.53654E-03 ZE 1.54532E-09
Constitution:      SiteFraction      Molality      Activity      log10Act
H2O                9.96927E-01      5.55084E+01    9.96605E-01    -0.0015
CL-1               1.53654E-03      8.55538E-02    6.73425E-02    -1.1717
NA+1               1.53654E-03      8.55538E-02    6.73424E-02    -1.1717
H+1               2.37132E-09      1.32034E-07    1.04050E-07    -6.9828
OH-1              2.19965E-09      1.22476E-07    9.63757E-08    -7.0160
O2                4.70270E-10      2.61844E-08    2.61828E-08    -7.5820
O3                1.00000E-12      0.00000E+00    2.70935E-38    -37.5671
HClO              1.00000E-12      0.00000E+00    3.25360E-20    -19.4876
H2O2              1.00000E-12      0.00000E+00    3.68420E-21    -20.4337
HClO2             1.00000E-12      0.00000E+00    1.28717E-37    -36.8904
H2                1.00000E-12      0.00000E+00    5.39110E-43    -42.2683
HO2-1            1.00000E-12      0.00000E+00    7.49315E-26    -25.1253
ClO4-1           1.00000E-12      0.00000E+00    8.09139E-33    -32.0920
ClO3-1           1.00000E-12      0.00000E+00    1.41605E-30    -29.8489
ClO2-1           1.00000E-12      0.00000E+00    1.29472E-32    -31.8878
ClO2              1.00000E-12      0.00000E+00    4.84011E-38    -37.3151
ClO-1             1.00000E-12      0.00000E+00    6.77886E-21    -20.1688
CL2              1.00000E-12      0.00000E+00    4.80004E-25    -24.3188
Solution Properties: pH = 6.9828 Eh = 0.7417 V I = 0.0856
pe = 12.5375 Ah = 71.5647 kJ m* = 0.1711
Aw = 0.9966 Os = 1.1033 pKw = 13.9973
At1= 1.0000E-12 At2= 1.2248E-07 (equiv_mol/kg_H2O)

POLY_3: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE      STATUS      DRIVING FORCE      MOLES
AQUEOUS      ENTERED      0.000000E+00      5.567954E+01
SUSPENDED PHASES:
REF ELECTRODE NAOH_S2 NAOH NAO2 NA2O_S3 NA2O_S2 NA2O2_S2 NA2O2 NA2O HCP_A3
HALITE FCC_A1 BCC_A2 AQUEOUS#3 AQUEOUS#2 GAS
POLY_3: sh b n n(*)
... the command in full is SHOW_VALUE
B=1005.
N=55.679543
N(H2O)=55.508435, N(H+1)=-9.7239338E-8, N(ZE)=8.6042549E-8,
N(NA)=8.5553782E-2, N(CL)=8.5553803E-2
POLY_3:Hit RETURN to continue
POLY_3:
POLY_3: @@... Calculating an equilibrium with all phases presented:
POLY_3: @@ (except for REF_ELE)
POLY_3: c-st p *=ent 0
... the command in full is CHANGE_STATUS
POLY_3: c-st p AQUEOUS=ent 55.8
... the command in full is CHANGE_STATUS
POLY_3: @@ ..... Always setting the REF ELECTRODE phase as SUSPENDED:
POLY_3: c-st p REF_ELE=sus
... the command in full is CHANGE_STATUS
POLY_3: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE      STATUS      DRIVING FORCE      MOLES
NAOH_S2      ENTERED      0.000000E+00      0.000000E+00
NAOH          ENTERED      0.000000E+00      0.000000E+00
NAO2          ENTERED      0.000000E+00      0.000000E+00
NA2O_S3       ENTERED      0.000000E+00      0.000000E+00
NA2O_S2       ENTERED      0.000000E+00      0.000000E+00
NA2O2_S2      ENTERED      0.000000E+00      0.000000E+00
NA2O2         ENTERED      0.000000E+00      0.000000E+00
NA2O          ENTERED      0.000000E+00      0.000000E+00
HCP_A3        ENTERED      0.000000E+00      0.000000E+00
HALITE        ENTERED      0.000000E+00      0.000000E+00
FCC_A1        ENTERED      0.000000E+00      0.000000E+00
BCC_A2        ENTERED      0.000000E+00      0.000000E+00
AQUEOUS#3     ENTERED      0.000000E+00      0.000000E+00
AQUEOUS#2     ENTERED      0.000000E+00      0.000000E+00
AQUEOUS       ENTERED      0.000000E+00      5.580000E+01
GAS           ENTERED      0.000000E+00      0.000000E+00
SUSPENDED PHASES:
REF ELECTRODE
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 679 grid points in 0 s
Found the set of lowest grid points in 0 s
Calculated POLY solution 1 s, total time 1 s
POLY_3: l-e ,x
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: PAQ2

Conditions:
P=1E5, T=298.15, B(H2O)=1000, B(NA)=1.96686, B(CL)=3.03314, N(H+1)=0,
N(ZE)=0
DEGREES OF FREEDOM 0

Temperature 298.15 K ( 25.00 C), Pressure 1.000000E+05
Number of moles of components 5.56795E+01, Mass in grams 1.00500E+03
Total Gibbs energy -1.70630E+07, Enthalpy -1.59010E+07, Volume 0.00000E+00

Component      Moles      M-Fraction  Activity  Potential  Ref.stat
H2O             5.5508E+01  9.9693E-01  9.9654E-01 -8.5871E+00 AQUEOUS

```

```
H+1          -9.7239E-08 -1.7464E-09 1.0405E-07 -3.9858E+04 SER
ZE           8.6043E-08  1.5453E-09 3.4476E+12  7.1565E+04 REF_ELEC
NA           8.5554E-02  1.5365E-03 4.5046E-63 -3.5588E+05 SER
CL           8.5554E-02  1.5365E-03 4.1623E-18 -9.9210E+04 SER
```

```
AQUEOUS                      Status ENTERED      Driving force 0.0000E+00
Moles 5.5680E+01, Mass 1.0050E+03, Volume fraction 0.0000E+00 Mole fractions:
H2O 9.96927E-01 NA 1.53654E-03 H+1 -1.74641E-09
CL 1.53654E-03 ZE 1.54532E-09
Constitution:
H2O 9.96927E-01 5.55084E+01 9.96605E-01 -0.0015
CL-1 1.53654E-03 8.55538E-02 6.73425E-02 -1.1717
NA+1 1.53654E-03 8.55538E-02 6.73424E-02 -1.1717
H+1 2.37132E-09 1.32034E-07 1.04050E-07 -6.9828
OH-1 2.19965E-09 1.22476E-07 9.63757E-08 -7.0160
O2 4.70270E-10 2.61844E-08 2.61828E-08 -7.5820
O3 1.00000E-12 0.00000E+00 2.70935E-38 -37.5671
HClO 1.00000E-12 0.00000E+00 3.25360E-20 -19.4876
H2O2 1.00000E-12 0.00000E+00 3.68420E-21 -20.4337
HClO2 1.00000E-12 0.00000E+00 1.28717E-37 -36.8904
H2 1.00000E-12 0.00000E+00 5.39110E-43 -42.2683
HO2-1 1.00000E-12 0.00000E+00 7.49315E-26 -25.1253
ClO4-1 1.00000E-12 0.00000E+00 8.09139E-33 -32.0920
ClO3-1 1.00000E-12 0.00000E+00 1.41605E-30 -29.8489
ClO2-1 1.00000E-12 0.00000E+00 1.29472E-32 -31.8878
ClO2 1.00000E-12 0.00000E+00 4.84011E-38 -37.3151
ClO-1 1.00000E-12 0.00000E+00 6.77886E-21 -20.1688
Cl2 1.00000E-12 0.00000E+00 4.80004E-25 -24.3188
Solution Properties: pH = 6.9828 Eh = 0.7417 V I = 0.0856
pe = 12.5375 Ah = 71.5647 kJ m* = 0.1711
Aw = 0.9966 Os = 1.1033 pKw = 13.9973
At1= 1.0000E-12 At2= 1.2248E-07 (equiv_mol/kg_H2O)
```

```
POLY_3: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE STATUS DRIVING FORCE MOLES
AQUEOUS#3 ENTERED 0.000000E+00 0.000000E+00
AQUEOUS#2 ENTERED 0.000000E+00 0.000000E+00
AQUEOUS ENTERED 0.000000E+00 5.567954E+01
GAS ENTERED -3.453482E+00 0.000000E+00
HALITE ENTERED -4.519288E+00 0.000000E+00
NAOH ENTERED -1.737487E+01 0.000000E+00
BCC_A2 ENTERED -1.752962E+01 0.000000E+00
FCC_A1 ENTERED -1.752962E+01 0.000000E+00
NAOH_S2 ENTERED -1.793977E+01 0.000000E+00
NAO2 ENTERED -1.999496E+01 0.000000E+00
NA2O2 ENTERED -2.605088E+01 0.000000E+00
NA2O2_S2 ENTERED -2.640940E+01 0.000000E+00
NA2O ENTERED -4.241247E+01 0.000000E+00
ENTERED PHASES WITH DRIVING FORCE LESS THAN -4.257992E+01
NA2O_S2 NA2O_S3 HCP_A3
SUSPENDED PHASES:
REF ELECTRODE
```

```
POLY_3: sh b n n(*)
... the command in full is SHOW_VALUE
B=1005.
N=55.679543
N(H2O)=55.508435, N(H+1)=-9.7239338E-8, N(ZE)=8.6042557E-4,
N(NA)=8.5553782E-2, N(CL)=8.5553803E-2
```

```
POLY_3: @@
POLY_3: @@ As shown here, 0.5wt% of NaCl (in 1 kg of H2O) is equivalent to
POLY_3: @@ 0.085554 molality of NaCl.
POLY_3: @@
POLY_3:
POLY_3: @@... Saving the workspace for the H2O-NaCl system:
POLY_3: save TCEX53.a.POLY3 y
... the command in full is SAVE_WORKSPACES
POLY_3:Hit RETURN to continue
```

```
POLY_3:
POLY_3: @@ =====
POLY_3: @@ Step 2: Single-Point Calculations for Fe-X (X = Cr-Ni-Co) system
POLY_3: @@ *****
POLY_3: @@ To demonstrate how to define the initial amount of alloy
POLY_3: @@ in an aqueous-bearing heterogeneous interaction system:
POLY_3: @@ -----
POLY_3: @@ Note: We are interested in only the BCC_A2 and FCC_A1 phases in
POLY_3: @@ the Fe-based alloy, in the current testing calculation.
POLY_3: @@ One may consider other possible phases (which exist in the
POLY_3: @@ applied steel material) if necessary.
POLY_3: @@
```

```
POLY_3: go data
... the command in full is GOTO_MODULE
```

```
TDB_PAQ2: rej sys
... the command in full is REJECT
H O ZE
VA DEFINED
LIQUID:L REJECTED
GRAPHITE DIAMOND_A4 FC_ORTHORHOMBIC
MONOCLINIC REJECTED
CBCC_A12 CUB_A13 CHI_A12
FE4N FECL2 REJECTED
CEMENTITE M23C6 M7C3
M5C2 M3C2 KSI_CARBIDE
PI REJECTED
FE3C NI3C CR3C2
CR7C3 CR23C6 REJECTED
COCO3 FECL3 NAHCO3
NA2CO3 NA2CO3_S2 NICO3
CRC606 REJECTED
CO3N CRN CR2N
FE2N NI3N REJECTED
NANO2 NANO2_S2 NANO3
REJECTED
COCL2 CRCL2 CRCL3
FECL2 FECL3 NICKL2
REJECTED
FECLO NACL04 NACL04_S2
REJECTED
REINITIATING GES5 .....
```

```
TDB_PAQ2: sw PAQ2
... the command in full is SWITCH_DATABASE
TDB_PAQ2: rej ele H O ZE
... the command in full is REJECT
H O ZE
```

```

REJECTED
TDB_PAQ2: d-sys Fe Cr Ni Co
... the command in full is DEFINE_SYSTEM
FE              CR              NI
CO DEFINED
TDB_PAQ2: l-sys const
... the command in full is LIST_SYSTEM
GAS:G           :CO CR CR2 FE NI:
> Gaseous Mixture, using the ideal gas model
FCC A1          :CO CR FE NI:VA:
> This is also the MX (X=C,N) solution phase.
BCC A2          :CO CR FE NI:VA:
> This is also the MX3 (X=C,N) solution phase.
HCP A3          :CO CR FE NI:VA:
> This is also the M2X (X=C,N) solution phase.
SIGMA          :CO FE NI:CR:CO CR FE NI:
TDB_PAQ2: rej-ph *
... the command in full is REJECT
GAS:G           FCC_A1          BCC_A2
HCP A3          SIGMA REJECTED
TDB_PAQ2: rest-ph FCC_A1 BCC_A2
... the command in full is RESTORE
FCC_A1          BCC_A2 RESTORED
TDB_PAQ2: get
... the command in full is GET_DATA
REINITIATING GES5 .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

'TCS public data set for liquid mixture and alloy solutions in the Fe-Co
-Cr-Na-Ni-C-H-O-N-S-Cl system.'
-OK-
TDB_PAQ2:Hit RETURN to continue
TDB_PAQ2:
TDB_PAQ2: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3:
POLY_3: @@... One may turn on the Global Minimization in the calculations:
POLY_3: Adv-Opt EQ_CALC Y Y !
... the command in full is ADVANCED_OPTIONS
Settings for the minimization of an equilibra:
POLY_3: Adv-Opt GLOBAL Y 20000 !
... the command in full is ADVANCED_OPTIONS
Settings for global minimization:
POLY_3:
POLY_3: s-c P=1e5 T=298.15
... the command in full is SET_CONDITION
POLY_3:
POLY_3: @@... The following conditions [system-size B and initial bulk
POLY_3: @@ composition w(i) of Fe-alloy] corresponds to the total
POLY_3: @@ initial amount of Fe-based alloy in the interaction,
POLY_3: @@ i.e., 1 gram of steel (Fe-10Cr-5Ni-1Co wt%).
POLY_3: s-c B=1 w(Cr)=.10 w(Ni)=.05 w(Co)=.01
... the command in full is SET_CONDITION
POLY_3:
POLY_3: l-c
... the command in full is LIST_CONDITIONS
P=1E5, T=298.15, B=1, W(CR)=0.1, W(NI)=5E-2, W(CO)=1E-2
DEGREES OF FREEDOM 0
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated 39296 grid points in 0 s
Found the set of lowest grid points in 0 s
Creating a new composition set BCC_A2#2
Calculated POLY solution 0 s, total time 0 s
POLY_3: l-e ,x
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: PAQ2

Conditions:
P=1E5, T=298.15, B=1, W(CR)=0.1, W(NI)=5E-2, W(CO)=1E-2
DEGREES OF FREEDOM 0

Temperature 298.15 K ( 25.00 C), Pressure 1.000000E+05
Number of moles of components 1.79859E-02, Mass in grams 1.00000E+00
Total Gibbs energy -1.58616E+02, Enthalpy -1.09889E+01, Volume 1.20553E-07

Component      Moles      M-Fraction Activity Potential Ref.stat
CO              1.6968E-04  9.4342E-03 4.4157E-08 -4.1983E+04 SER
CR              1.9232E-03  1.0693E-01 5.8926E-02 -7.0192E+03 SER
FE              1.5041E-02  8.3627E-01 3.7073E-02 -8.1679E+03 SER
NI              8.5193E-04  4.7367E-02 7.7089E-04 -1.7769E+04 SER

BCC_A2#2              Status ENTERED Driving force 0.0000E+00
Moles 1.4641E-02, Mass 8.1821E-01, Volume fraction 8.5170E-01 Mole fractions:
FE 9.87131E-01 CO 1.15888E-02 NI 8.17873E-04 CR 4.61992E-04

BCC A2              Status ENTERED Driving force 0.0000E+00
Moles 1.9166E-03, Mass 9.9654E-02, Volume fraction 1.1495E-01 Mole fractions:
CR 9.99946E-01 FE 5.39522E-05 CO 9.25541E-12 NI 8.81026E-12

FCC A1              Status ENTERED Driving force 0.0000E+00
Moles 1.4280E-03, Mass 8.2138E-02, Volume fraction 3.3346E-02 Mole fractions:
NI 5.88202E-01 FE 4.11792E-01 CO 5.30943E-06 CR 6.98908E-09
POLY_3: l-st cp
... the command in full is LIST_STATUS
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS      REF. STATE      T(K)              P(Pa)
VA              ENTERED      SER
CO              ENTERED      SER
CR              ENTERED      SER
FE              ENTERED      SER
NI              ENTERED      SER
*** STATUS FOR ALL PHASES
PHASE              STATUS      DRIVING FORCE      MOLES

```

```

FCC_A1          ENTERED      0.000000E+00   1.428010E-03
BCC_A2#2        ENTERED      0.000000E+00   1.464136E-02
BCC_A2          ENTERED      0.000000E+00   1.916564E-03
POLY_3: sh b n n(*)
... the command in full is SHOW_VALUE
B=1.
N=1.7985937E-2
N(CO)=1.6968364E-4, N(CR)=1.9232249E-3, N(FE)=1.5041094E-2, N(NI)=8.5193389E-4
POLY_3:Hit RETURN to continue
POLY_3:
POLY_3: s-c T=1073.15
... the command in full is SET_CONDITION
POLY_3: l-c
... the command in full is LIST_CONDITIONS
P=1E5, T=1073.15, B=1, W(CR)=0.1, W(NI)=5E-2, W(CO)=1E-2
DEGREES OF FREEDOM 0
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Using global minimization procedure
Calculated      39296 grid points in          1 s
Found the set of lowest grid points in          0 s
Calculated POLY solution      0 s, total time    1 s
POLY_3: l-e ,x
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium =      1, label A0 , database: PAQ2

Conditions:
P=1E5, T=1073.15, B=1, W(CR)=0.1, W(NI)=5E-2, W(CO)=1E-2
DEGREES OF FREEDOM 0

Temperature  1073.15 K ( 800.00 C), Pressure  1.000000E+05
Number of moles of components 1.79859E-02, Mass in grams 1.00000E+00
Total Gibbs energy -9.18150E+02, Enthalpy 5.59649E+02, Volume 1.23044E-07

Component      Moles      M-Fraction Activity Potential Ref.stat
CO              1.6968E-04  9.4342E-03 1.8364E-05 -9.7303E+04 SER
CR              1.9232E-03  1.0693E-01 3.0133E-03 -5.1794E+04 SER
FE              1.5041E-02  8.3627E-01 4.2352E-03 -4.8757E+04 SER
NI              8.5193E-04  4.7367E-02 1.1925E-04 -8.0610E+04 SER

FCC_A1          Status ENTERED      Driving force 0.0000E+00
Moles 1.7986E-02, Mass 1.0000E+00, Volume fraction 1.0000E+00 Mole fractions:
FE 8.36270E-01 CR 1.06929E-01 NI 4.73667E-02 CO 9.43424E-03
POLY_3: l-st cp
... the command in full is LIST_STATUS
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS      REF. STATE      T(K)          P(Pa)
VA              ENTERED      SER
CO              ENTERED      SER
CR              ENTERED      SER
FE              ENTERED      SER
NI              ENTERED      SER
*** STATUS FOR ALL PHASES
PHASE          STATUS      DRIVING FORCE      MOLES
FCC_A1          ENTERED      0.000000E+00      1.798594E-02
BCC_A2#2        ENTERED      -1.564120E-02      0.000000E+00
BCC_A2          ENTERED      -1.564120E-02      0.000000E+00
POLY_3: sh b n n(*)
... the command in full is SHOW_VALUE
B=1.
N=1.7985937E-2
N(CO)=1.6968364E-4, N(CR)=1.9232249E-3, N(FE)=1.5041094E-2, N(NI)=8.5193389E-4
POLY_3: @@
POLY_3: @@ As shown here, 1 gram of steel (Fe-10Cr-5Ni-1Co wt%)
POLY_3: @@ is equivalent to:
POLY_3: @@ n(Fe) = 1.5041094E-2
POLY_3: @@ n(Cr) = 1.9232249E-3
POLY_3: @@ n(Ni) = 8.5193389E-4
POLY_3: @@ n(Co) = 1.6968422E-4
POLY_3: @@
POLY_3: @@... Saving the workspace for the Fe-Cr-Ni-Co system:
POLY_3: save TCEX53_b.POLY3 y
... the command in full is SAVE_WORKSPACES
POLY_3:Hit RETURN to continue
POLY_3:
POLY_3: @@ =====
POLY_3: @@ Step 3: Single-Point Calculations for Fe-Cr-Ni-Co + H2O-NaCl system
POLY_3: @@ *****
POLY_3: @@ Bulk composition in the heterogeneous interaction system:
POLY_3: @@ b(H2O) = 1000
POLY_3: @@ n(NaCl) = 0.085554
POLY_3: @@ n(Fe) = 1.5041094E-2
POLY_3: @@ n(Cr) = 1.9232249E-3
POLY_3: @@ n(Ni) = 8.5193389E-4
POLY_3: @@ n(Co) = 1.6968422E-4
POLY_3:
POLY_3: @@... Retrieving data from the PAQ2 or PAQS2 database:
POLY_3: go data
... the command in full is GOTO_MODULE
TDB_PAQ2: rej sys
... the command in full is REJECT
H              O              ZE
VA DEFINED
LIQUID:L REJECTED
GRAPHITE       DIAMOND_A4      FC_ORTHORHOMBIC
MONOCLINIC REJECTED
CBCC_A12       CUB_A13         CHI_A12
FE4N           FECN_CHI REJECTED
CEMENTITE      M23C6          M7C3
M5C2           M3C2           KSI_CARBIDE
PI REJECTED
FE3C           NI3C           CR3C2
CR7C3          CR23C6 REJECTED
COCO3          FECO3          NAHCO3
NA2CO3         NA2CO3_S2        NICO3
CRC6O6 REJECTED
CO3N           CRN           CR2N
FE2N           NI3N REJECTED
NANO2          NANO2_S2        NANO3
REJECTED
COCL2          CRCL2          CRCL3
FECL2          FECL3          NICL2
REJECTED

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FECLO                      NACLO4                      NACLO4_S2
REJECTED
REINITIATING GES5 .....
TDB_PAQ2: @@ ----- switch on PAQ2 or PAQS2
TDB_PAQ2: sw PAQ2
... the command in full is SWITCH_DATABASE
TDB_PAQ2: d-sys H O Na Cl Fe Cr Ni Co
... the command in full is DEFINE_SYSTEM
NA          CL          FE
CR          NI          CO
DEFINED
TDB_PAQ2: l-sys const
... the command in full is LIST_SYSTEM
AQUEOUS:A      :H2O H2 H+1 OH-1 H2O2 HO2-1 O2 O3 CO1H2O2 CL2 CL-1 CLO2 CLO-1
CLO2-1 CLO3-1 CLO4-1 HCLO HCLO2 CO+2 CO+3 CR+2 CR+3 CROH+2 CRO+1 CRO2-1
HCRO2 HCRO4-1 CRO4-2 CR2O7-2 FE+2 FE+3 FEOH+1 FEOH+2 FEO3H3-1 FE2O2H2+4
FECL+2 NA+1 NI+2 NIOH+1:
> Aqueous Solution: using the SIT Model (from TCAQ2 database)
REF_ELECTRODE :ZE:
> Reference Electrode for ZE potential; 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:
FE02H2          :FE1H2O2:
FE03H3          :FE1H3O3:
FE0OH           :FE1H1O2:
FE2O2O2H2       :FE2H2O4:
COO             :CO1O1:
CO3O4           :CO3O4:
COO2H2          :CO1H2O2:
CRO2            :CR1O2:
CRO3            :CR1O3:
CR2O3           :CR2O3:
CR5O12          :CR5O12:
CR8O21          :CR8O21:
NAO2            :NA1O2:
NA2O            :NA2O1:
NA2O_S2         :NA2O1:
NA2O_S3         :NA2O1:
NA2O2           :NA2O2:
NA2O2_S2        :NA2O2:
NAOH            :H1NA1O1:
NAOH_S2         :H1NA1O1:
NIO             :NI1O1:
NIO_S2          :NI1O1:
NIO2H2          :H2NI1O2:
NIOOH           :H1NI1O2:
FECR2O4         :CR2FE1O4:
COCR2O4         :CO1CR2O4:
NICR2O4         :CR2NI1O4:
NA2CR2O4        :CR2NA2O4:
COFE2O4         :CO1FE2O4:
NIFE2O4         :FE2NI1O4:
NA2CRO4         :CR1NA2O4:
NA2CRO4_S2      :CR1NA2O4:
NA2FEO2         :FE1NA1O2:
TDB_PAQ2:Hit RETURN to continue
TDB_PAQ2:
TDB_PAQ2: rej ph HCP_A3 CBCC_A12 CUB_A13 CHI_A12 Fe4N
... the command in full is REJECT
HCP_A3 REJECTED
TDB_PAQ2: rej ph SIGMA
... the command in full is REJECT
SIGMA REJECTED
TDB_PAQ2: rej ph NaH
... the command in full is REJECT
TDB_PAQ2: get
... the command in full is GET_DATA
REINITIATING GES5 .....
ELEMENTS .....
SPECIES .....
PHASES .....
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
... the command in full is AMEND_PHASE_DESCRIPTION
PARAMETERS ...
FUNCTIONS ....

List of references for assessed data

'TCS public data set for gaseous mixture in the Fe-Co-Cr-Na-Ni-C-H-O-N-S
-Cl system.'
'TCS public data set for liquid mixture and alloy solutions in the Fe-Co
-Cr-Na-Ni-C-H-O-N-S-Cl system.'
'TCS public data set for stoichiometric solids and liquids in the Fe-Co-Cr
-Na-Ni-C-H-O-N-S-Cl system.'
'TCS Aqueous Solution Database, TCAQ2, v2.0 (2002/2003). Extracted data
only for Fe-Co-Cr-Na-Ni-C-H-O-N-S-Cl bearing aqueous solution species
from TCAQ2 which covers totally 83 elements and contains many more
aqueous solution species.'
-OK-
TDB_PAQ2:Hit RETURN to continue
TDB_PAQ2:
TDB_PAQ2: @@... Defining system-components and their proper reference states:

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TDB_PAQ2: go p-3
... the command in full is GOTO_MODULE

POLY version 3.32
POLY_3: d-com H2O H+1 ZE Na Cl Fe Cr Ni Co
... the command in full is DEFINE_COMPONENTS
POLY_3: s-r-s H2O AQUEOUS * 1e5
... the command in full is SET_REFERENCE_STATE
POLY_3: s-r-s ZE REF_ELE * 1e5
... the command in full is SET_REFERENCE_STATE
POLY_3: l-st c
... the command in full is LIST_STATUS
*** STATUS FOR ALL COMPONENTS
COMPONENT      STATUS      REF. STATE      T(K)              P(Pa)
VA              ENTERED      SER
H2O             ENTERED      AQUEOUS          *              100000
H+1             ENTERED      SER
ZE              ENTERED      REF_ELECTRODE    *              100000
NA              ENTERED      SER
CL              ENTERED      SER
FE              ENTERED      SER
CR              ENTERED      SER
NI              ENTERED      SER
CO              ENTERED      SER
POLY_3:
POLY_3: @@... Defining some symbols (constants/variables/functions/tables):
POLY_3: @@ *****
POLY_3: @@ One may choose to just define some important ones as shown here,
POLY_3: @@ e.g., RNF; pH, Eh
POLY_3: @@ =====
POLY_3: @@ Important: With the default reference state (SER) used for
POLY_3: @@ system-component H+1, the pH condition in aqueous solution
POLY_3: @@ should be defined as below:
POLY_3: @@ pH = -log10[act(H+1,aqs)] (traditional)
POLY_3: @@ = -log10[acr(H+1,AQUEOUS)*55.508435] (Thermo-Calc)
POLY_3: @@ = -ln[acr(H+1,AQUEOUS)*55.508435]*2.302585093
POLY_3: @@ where
POLY_3: @@ act(H+1,aqs) is molality_based activity of
POLY_3: @@ H+1 species (as of the traditional concept);
POLY_3: @@ acr(H+1,AQ)*AH2O is site-fraction_based activity of
POLY_3: @@ H+1 species (calculated in Thermo-Calc).
POLY_3: @@
POLY_3: @@ Such a definition not only gives correct pH values for all
POLY_3: @@ thermodynamic models (SIT and HKF) but also does not affect
POLY_3: @@ the calculation of ACR(H+1) [LNACR(H+1)] quantity that is
POLY_3: @@ normally used as MAPPING/STEPPING variables in all modules
POLY_3: @@ (POURBAIX & TDB/GESS/POLY3/POST).
POLY_3: @@
POLY_3: @@ -----
POLY_3: @@ Notes:
POLY_3: @@ If desired, one may also choose to define many other possible
POLY_3: @@ symbols (for the convenience of plotting) on the same scope
POLY_3: @@ of the POURBAIX-Module.
POLY_3: @@
POLY_3: @@ A complete list of valid symbols for the Fe-Cr-Ni-Co-H2O-NaCl
POLY_3: @@ heterogeneous interaction system on the scope same as the
POLY_3: @@ automatically-defined symbols in the POURBAIX-Module can be
POLY_3: @@ found at the end of this MACRO file (only as a reference!).
POLY_3: @@
POLY_3: @@ Please pay attention to the followings:
POLY_3: @@ * AH2O is always a constant, and YH2O is the site fraction
POLY_3: @@ of the solvent H2O, i.e.,
POLY_3: @@ AH2O = 55.508435
POLY_3: @@ YH2O = Y(AQ,H2O)
POLY_3: @@
POLY_3: @@ * The AYT and ART quantities are on the Site-Fraction basis:
POLY_3: @@ AYT for AC(i,AQ)
POLY_3: @@ ART for ACR(i,AQ)
POLY_3: @@
POLY_3: @@ * The AIT (Aii), RCT (RCi) and MLT (MLi) quantities are
POLY_3: @@ on the Molality basis:
POLY_3: @@ AIT for ACR(i,AQ)*AH2O
POLY_3: @@ as activity based on molality
POLY_3: @@ RCT for ACR(i,AQ)*YH2O/Y(AQ,i)
POLY_3: @@ as activity coefficient based on molality
POLY_3: @@ MLT for Y(AQ,i)*AH2O/YH2O
POLY_3: @@ as molality
POLY_3: @@ -----
POLY_3: @@ Aii = RCi * MLi
POLY_3: @@ = ACR(i,AQ)*YH2O/Y(AQ,i) * Y(AQ,i)*AH2O/YH2O
POLY_3: @@ = ACR(i,AQ)*AH2O
POLY_3: @@
POLY_3: @@ * It is always ACR(sp,AQ) = AC(sp,AQ)
POLY_3: @@
POLY_3: @@ * It is always the Aii=AIT(H+1) [=ACR(H+1,AQ)*AH2O] quantity,
POLY_3: @@ rather than ART(H+1) [=ACR(H+1,AQ)] quantity, that is
POLY_3: @@ the equivalent property for the acidity condition pH.
POLY_3: @@ -----
POLY_3: @@
POLY_3: ent-sym const AH2O=55.508435
... the command in full is ENTER_SYMBOL
POLY_3: ent-sym const RNF =96485.309
... the command in full is ENTER_SYMBOL
POLY_3: ent-sym funct Eh = mur(ZE)/RNF;
... the command in full is ENTER_SYMBOL
POLY_3: ent-sym funct pH = -log10(acr(H+1,AQUEOUS)*AH2O);
... the command in full is ENTER_SYMBOL
POLY_3: l-sym
... the command in full is LIST_SYMBOLS
DEFINED CONSTANTS
AH2O=55.508435, RNF=96485.309
DEFINED FUNCTIONS AND VARIABLES%
EH=MUR(ZE)/RNF
PH=- LOG10(ACR(H+1,AQUEOUS)*AH2O )
POLY_3:
POLY_3: @@... Defining the equilibrium conditions:
POLY_3: @@ -----
POLY_3: @@ Defining P-T and bulk composition in the interaction system
POLY_3: @@ for calculating starting point [at e.g pH=7 & Eh=0 (V)]:
POLY_3: @@
POLY_3:

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POLY_3: @@ ----- P-T conditions:
POLY_3: s-c P=1e5 T=298.15
... the command in full is SET_CONDITION
POLY_3: @@
POLY_3: @@ ... Alternatively, it can be manually input as below:
POLY_3: @@ s-c P=
POLY_3: @@ @?Pressure_in_Pascal:
POLY_3: @@ s-c T=
POLY_3: @@ @?Temperature_In_Kelvin:
POLY_3:
POLY_3: @@ ----- For Aqueous-involving interaction system, it is always
POLY_3: @@ recommended to define 1 kg of H2O, so that it is very
POLY_3: @@ convenient to consider molality quantities and other
POLY_3: @@ properties in aqueous solution.
POLY_3: s-c b(H2O)=1000
... the command in full is SET_CONDITION
POLY_3:
POLY_3: @@ ----- The following is equivalent to 0.085554 mole of NaCl
POLY_3: @@ in 1 kg of H2O:
POLY_3: s-c n(Na)=0.085554 n(Cl)=0.085554
... the command in full is SET_CONDITION
POLY_3:
POLY_3: @@ ----- For calculating Pourbaix diagrams or other diagrams in
POLY_3: @@ aqueous-involving interaction system, it is important
POLY_3: @@ to consider the so-called "effective interaction rate".
POLY_3: @@
POLY_3: @@ The following is equivalent to 1 gram of specified steel
POLY_3: @@ (Fe-10Cr-5Ni-1Co wt%) in an effective interaction with
POLY_3: @@ 1 kg of H2O (dissolving 0.085554 mole of NaCl):
POLY_3: s-c n(Fe)=1.5041094E-2 n(Cr)=1.9232249E-3
... the command in full is SET_CONDITION
POLY_3: s-c n(Ni)=8.5193389E-4 n(Co)=1.6968422E-4
... the command in full is SET_CONDITION
POLY_3:
POLY_3: @@ ----- Let's calculate initial equilibrium at pH=7 & Eh=0 (V):
POLY_3: s-c lnacr(H+1)=-16.11809565 mur(ZE)=0
... the command in full is SET_CONDITION
POLY_3:
POLY_3: l-c
... the command in full is LIST_CONDITIONS
P=1E5, T=298.15, B(H2O)=1000, N(NA)=8.5554E-2, N(CL)=8.5554E-2,
N(Fe)=1.50411E-2, N(CR)=1.92322E-3, N(NI)=8.51934E-4, N(CO)=1.69684E-4,
LNACR(H+1)=-16.1181, MUR(ZE)=0
DEGREES OF FREEDOM 0
POLY_3:
POLY_3: @@ =====
POLY_3: @@... Turn off GLOBAL completely for aqueous calculations!
POLY_3: @@ -----
POLY_3: @@ Adv-Opt GLOBAL
POLY_3: @@ Use global minimization as much as possible /N/: N
POLY_3: @@ Use global minimization for test only? /N/: N
POLY_3: @@ -----
POLY_3: @@
POLY_3: Adv-Opt GLOBAL N N !
... the command in full is ADVANCED_OPTIONS
Settings for global minimization:
POLY_3: @@ -----
POLY_3: @@ Adv-Opt EQ_CALC
POLY_3: @@ Force positive definite phase Hessian /Y/: N
POLY_3: @@ Control stepsize during minimization /Y/: Y
POLY_3: @@ -----
POLY_3: Adv-Opt EQ_CALC N Y !
... the command in full is ADVANCED_OPTIONS
Settings for the minimization of an equilibra:
POLY_3:
POLY_3: @@ =====
POLY_3: @@... Setting numerical limits:
POLY_3: @@ -----
POLY_3: @@ Notes:
POLY_3: @@ For equilibrium calculations (single-point, stepping or mapping)
POLY_3: @@ of complex aqueous-bearing heterogeneous interaction systems,
POLY_3: @@ it is recommended to properly modify the numerical limits.
POLY_3: @@ The following command (changing the numerical limits from the
POLY_3: @@ default values "500 1E-6 1E-12 N" to "20000 1E-6 1E-20 Y")
POLY_3: @@ will bring the following changes:
POLY_3: @@ 1) The change on "Maximum number of iterations" from the
POLY_3: @@ default value 500 to 20000, which enforces 40 times
POLY_3: @@ more iterations for each of the calculations in order
POLY_3: @@ to obtain stable equilibria;
POLY_3: @@ 2) The "Required accuracy" remains the default value 1E-6.
POLY_3: @@ It may be changed to 1E-4, that will allow less accurate
POLY_3: @@ calculations and thus make it easier/faster to converge;
POLY_3: @@ 3) The change on "Smallest fraction" from the default site
POLY_3: @@ fraction of 1E-12 to 1E-20, that is more suitable for
POLY_3: @@ for aqueous solution phase; and
POLY_3: @@ 4) The "Approximate driving force for metastable phases" option
POLY_3: @@ is changed from the default value of "N" to "Y" (meaning
POLY_3: @@ it should always approximately calculate driving forces
POLY_3: @@ for metastable phases).
POLY_3: @@ Such changes in the numerical limits are essential and useful
POLY_3: @@ for making sure of finding a converged solution of stable
POLY_3: @@ equilibria, especially when the heterogeneous interaction
POLY_3: @@ system becomes more and more complicated.
POLY_3: @@ -----
POLY_3: @@
POLY_3: s-n-l 20000 1e-6 1e-20 Y
... the command in full is SET_NUMERICAL_LIMITS
LIMITATIONS of the present version of Thermo-Calculations
Max number of elements : 40
Max number of species :5000
Max number of sublattices in a phase : 10
Max number of constituents in a phase: : 200

Max number of constituents in an ideal phase :5000

POLY_3:
POLY_3:
POLY_3: @@... Calculating an equilibrium with only AQUEOUS presented:
POLY_3: c-st p *=sus

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... the command in full is CHANGE_STATUS
POLY_3: c-st p AQUEOUS=ent 55.8
... the command in full is CHANGE_STATUS
POLY_3: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE          STATUS      DRIVING FORCE    MOLES
AQUEOUS        ENTERED    0.000000E+00    6.138000E+03
SUSPENDED PHASES:
WUSTITE REF ELECTRODE NIO_S2 NIOOH NIO2H2 NIO NIFE2O4 NICR2O4 NAOH_S2 NAOH
NAO2 NA2O_S3 NA2O_S2 NA2O2_S2 NA2O2 NA2O NA2FEO2 NA2CRO4_S2 NA2CRO4 NA2CR2O4
MAGNETITE HEMATITE HALITE FEOOH FEO3H3 FEO2H2 FECR2O4 FE2O3 GAMMA FE2O2O2H2
FCC_A1 CRO3 CRO2 CR8O21 CR5O12 CR2O3 COO2H2 COO COFE2O4 COCR2O4 CO3O4 BCC_A2
GAS
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM
Global equilibrium calculation turned off, you can turn it on with
ADVANCED_OPTIONS GLOBAL_MINIMIZATION Y,,,,,,,,,
109 ITS, CPU TIME USED 0 SECONDS
POLY_3: l-e ,x
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: PAQ2

Conditions:
P=1E5, T=298.15, B(H2O)=1000, N(NA)=8.5554E-2, N(CL)=8.5554E-2,
N(FE)=1.5041E-2, N(CR)=1.92322E-3, N(NI)=8.51934E-4, N(CO)=1.69684E-4,
LNACR(H+1)=-16.1181, MUR(ZE)=0
DEGREES OF FREEDOM 0

Temperature 298.15 K ( 25.00 C), Pressure 1.000000E+05
Number of moles of components 5.57254E+01, Mass in grams 1.00599E+03
Total Gibbs energy -1.70641E+07, Enthalpy -1.59024E+07, Volume -4.21624E-08

Component      Moles      M-Fraction Activity Potential Ref.stat
H2O             5.5508E+01  9.9611E-01  9.9606E-01 -9.7846E+00 AQUEOUS
H+1            -1.0027E-02 -1.7993E-04  1.0000E-07 -3.9956E+04 SER
ZE             3.7895E-02  6.8003E-04  1.0000E+00  0.0000E+00 REF_ELEC
NA             8.5554E-02  1.5353E-03  1.5211E-50 -2.8436E+05 SER
CL             8.5554E-02  1.5353E-03  1.1822E-30 -1.7083E+05 SER
FE             1.5041E-02  2.6991E-04  1.2285E-18 -1.0223E+05 SER
CR             1.9232E-03  3.4513E-05  1.6596E-45 -2.5561E+05 SER
NI             8.5193E-04  1.5288E-05  6.0058E-14 -7.5468E+04 SER
CO             1.6968E-04  3.0450E-06  3.2708E-16 -8.8391E+04 SER

AQUEOUS
Status ENTERED Driving force 0.0000E+00
Moles 5.5725E+01, Mass 1.0060E+03, Volume fraction 1.0000E+00 Mole fractions:
H2O 9.96107E-01 ZE 6.80033E-04 NI 1.52881E-05
CL 1.53528E-03 FE 2.69915E-04 CO 3.04501E-06
NA 1.53528E-03 CR 3.45125E-05 H+1 -1.79930E-04
Constitution: SiteFraction Molality Activity log10Act
H2O 9.96604E-01 5.55084E+01 9.96157E-01 -0.0017
CL-1 1.53628E-03 8.55668E-02 6.59412E-02 -1.1808
NA+1 1.53628E-03 8.55668E-02 6.59591E-02 -1.1807
FE+2 1.56791E-04 8.73285E-03 3.08751E-03 -2.5104
FEOH+1 1.13299E-04 6.31049E-03 4.86919E-03 -2.3125
CRO+1 3.00740E-05 1.67505E-03 1.29247E-03 -2.8886
NI+2 1.52852E-05 8.51348E-04 3.02381E-04 -3.5194
CROH+2 3.38456E-06 1.88512E-04 6.68399E-05 -4.1750
CO+2 3.04698E-06 1.69710E-04 6.02711E-05 -4.2199
HCRO2 1.05903E-06 5.89856E-05 5.89799E-05 -4.2293
NIOH+1 1.28111E-08 7.13548E-07 5.50574E-07 -6.2592
CR+3 1.12056E-08 6.24122E-07 6.07385E-08 -7.2165
CRO2-1 6.16631E-09 3.43448E-07 2.65005E-07 -6.5767
OH-1 2.33522E-09 1.30066E-07 1.00231E-07 -6.9990
H+1 2.32641E-09 1.29576E-07 1.00000E-07 -7.0000
FEOH+2 1.10316E-12 6.14435E-11 2.17858E-11 -10.6618
CR+2 1.47493E-16 8.21498E-15 2.91275E-15 -14.5357
FE+3 6.69156E-17 3.72704E-15 3.61605E-16 -15.4418
FECI+2 3.43228E-17 1.91170E-15 6.77823E-16 -15.1689
H2 1.06276E-19 5.91933E-18 5.91876E-18 -17.2278
FE2O2H2+4 2.32944E-20 1.29744E-18 2.05117E-20 -19.6880
O3 1.00000E-20 0.00000E+00 2.0444E-113 -112.6894
FEO3H3-1 1.00000E-20 0.00000E+00 4.15261E-44 -43.3817
H2O2 1.00000E-20 0.00000E+00 3.35251E-46 -45.4746
CRO4-2 1.00000E-20 0.00000E+00 1.67197E-26 -25.7768
HClO 1.00000E-20 0.00000E+00 2.78756E-45 -44.5548
HClO2 1.00000E-20 0.00000E+00 1.00400E-87 -86.9983
CRO2-2 1.00000E-20 0.00000E+00 9.28118E-52 -51.0324
HCRO4-1 1.00000E-20 0.00000E+00 5.05292E-27 -26.2965
HO2-1 1.00000E-20 0.00000E+00 7.09471E-51 -50.1491
CO1H2O2 1.00000E-20 0.00000E+00 5.9656E-101 -100.2243
CO+3 1.00000E-20 0.00000E+00 7.96270E-38 -37.0989
O2 1.00000E-20 0.00000E+00 2.17014E-58 -57.6635
CLO4-1 1.00000E-20 0.00000E+00 5.4430E-133 -132.2642
CLO3-1 1.00000E-20 0.00000E+00 1.0463E-105 -104.9803
CLO2-1 1.00000E-20 0.00000E+00 1.05079E-82 -81.9785
CLO2 1.00000E-20 0.00000E+00 1.1394E-100 -99.9433
CLO-1 1.00000E-20 0.00000E+00 6.04311E-46 -45.2187
CL2 1.00000E-20 0.00000E+00 3.87204E-50 -49.4121
Solution Properties: pH = 7.0000 Eh = 0.0000 V I = 0.1094
pe = 0.0000 Ah = 0.0000 kJ m* = 0.1891
Aw = 0.9962 Os = 1.1300 pKw = 13.9973
At1= 1.0000E-20 At2= 1.3007E-07 (equiv_mol/kg_H2O)

POLY_3: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE          STATUS      DRIVING FORCE    MOLES
AQUEOUS        ENTERED    0.000000E+00    5.572540E+01
SUSPENDED PHASES:
WUSTITE REF ELECTRODE NIO_S2 NIOOH NIO2H2 NIO NIFE2O4 NICR2O4 NAOH_S2 NAOH
NAO2 NA2O_S3 NA2O_S2 NA2O2_S2 NA2O2 NA2O NA2FEO2 NA2CRO4_S2 NA2CRO4 NA2CR2O4
MAGNETITE HEMATITE HALITE FEOOH FEO3H3 FEO2H2 FECR2O4 FE2O3 GAMMA FE2O2O2H2
FCC_A1 CRO3 CRO2 CR8O21 CR5O12 CR2O3 COO2H2 COO COFE2O4 COCR2O4 CO3O4 BCC_A2
GAS
POLY_3: sh b n n(*)
... the command in full is SHOW_VALUE
B=1005.9899
N=55.725397
N(H2O)=55.508435, N(H+1)=-1.0026646E-2, N(ZE)=3.7895099E-2, N(NA)=8.5554E-2,
N(CL)=8.5554E-2, N(FE)=1.5041094E-2, N(CR)=1.9232249E-3,
N(NI)=8.5193389E-4, N(CO)=1.6968422E-4
POLY_3:Hit RETURN to continuePOLY_3:
POLY_3: @@... Calculating an equilibrium with all phases presented:
POLY_3: @@ (except for REF_ELE)
POLY_3: c-st p *=ent 0

```



```

... the command in full is CHANGE_STATUS
POLY_3: c-st p AQUEOUS=ent 55.8
... the command in full is CHANGE_STATUS
POLY_3: @@ ..... Always setting the REF_ELECTRODE phase as SUSPENDED:
POLY_3: c-st p REF_ELE=sus
... the command in full is CHANGE_STATUS
POLY_3: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES

```

PHASE	STATUS	DRIVING FORCE	MOLES
WUSTITE	ENTERED	0.000000E+00	0.000000E+00
NIO_S2	ENTERED	0.000000E+00	0.000000E+00
NIOOH	ENTERED	0.000000E+00	0.000000E+00
NIO2H2	ENTERED	0.000000E+00	0.000000E+00
NIO	ENTERED	0.000000E+00	0.000000E+00
NIFE2O4	ENTERED	0.000000E+00	0.000000E+00
NICR2O4	ENTERED	0.000000E+00	0.000000E+00
NAOH_S2	ENTERED	0.000000E+00	0.000000E+00
NAOH	ENTERED	0.000000E+00	0.000000E+00
NAO2	ENTERED	0.000000E+00	0.000000E+00
NA2O_S3	ENTERED	0.000000E+00	0.000000E+00
NA2O_S2	ENTERED	0.000000E+00	0.000000E+00
NA2O2_S2	ENTERED	0.000000E+00	0.000000E+00
NA2O2	ENTERED	0.000000E+00	0.000000E+00
NA2O	ENTERED	0.000000E+00	0.000000E+00
NA2FEO2	ENTERED	0.000000E+00	0.000000E+00
NA2CRO4_S2	ENTERED	0.000000E+00	0.000000E+00
NA2CRO4	ENTERED	0.000000E+00	0.000000E+00
NA2CR2O4	ENTERED	0.000000E+00	0.000000E+00
MAGNETITE	ENTERED	0.000000E+00	0.000000E+00
HEMATITE	ENTERED	0.000000E+00	0.000000E+00
HALITE	ENTERED	0.000000E+00	0.000000E+00
FE0OH	ENTERED	0.000000E+00	0.000000E+00
FE03H3	ENTERED	0.000000E+00	0.000000E+00
FE02H2	ENTERED	0.000000E+00	0.000000E+00
FE0CR2O4	ENTERED	0.000000E+00	0.000000E+00
FE2O3_GAMMA	ENTERED	0.000000E+00	0.000000E+00
FE2O2O2H2	ENTERED	0.000000E+00	0.000000E+00
FCC_A1	ENTERED	0.000000E+00	0.000000E+00
CRO3	ENTERED	0.000000E+00	0.000000E+00
CRO2	ENTERED	0.000000E+00	0.000000E+00
CR8O21	ENTERED	0.000000E+00	0.000000E+00
CR5O12	ENTERED	0.000000E+00	0.000000E+00
CR2O3	ENTERED	0.000000E+00	0.000000E+00
COO2H2	ENTERED	0.000000E+00	0.000000E+00
COO	ENTERED	0.000000E+00	0.000000E+00
COFE2O4	ENTERED	0.000000E+00	0.000000E+00
COCR2O4	ENTERED	0.000000E+00	0.000000E+00
CO3O4	ENTERED	0.000000E+00	0.000000E+00
BCC_A2	ENTERED	0.000000E+00	0.000000E+00
AQUEOUS	ENTERED	0.000000E+00	5.583623E+01
GAS	ENTERED	0.000000E+00	0.000000E+00

```

SUSPENDED PHASES:
REF_ELECTRODE
POLY_3: c-e
... the command in full is COMPUTE_EQUILIBRIUM

79 ITS, CPU TIME USED 0 SECONDS
POLY_3: l-e ,x
... the command in full is LIST_EQUILIBRIUM
Output from POLY-3, equilibrium = 1, label A0 , database: PAQ2

Conditions:
P=1E5, T=298.15, B(H2O)=1000, N(NA)=8.5554E-2, N(CL)=8.5554E-2,
N(Fe)=1.50411E-2, N(CR)=1.92322E-3, N(NI)=8.51934E-4, N(CO)=1.69684E-4,
LNACR(H+1)=-16.1181, MUR(ZE)=0
DEGREES OF FREEDOM 0

Temperature 298.15 K ( 25.00 C), Pressure 1.000000E+05
Number of moles of components 5.56976E+01, Mass in grams 1.00595E+03
Total Gibbs energy -1.70627E+07, Enthalpy -1.59010E+07, Volume -3.10120E-16

Component      Moles      M-Fraction  Activity  Potential  Ref.stat
H2O             5.5508E+01  9.9660E-01  9.9654E-01 -8.5924E+00 AQUEOUS
H+1            -5.2910E-02 -9.4995E-04  1.0000E-07 -3.9956E+04 SER
ZE             5.2936E-02  9.5042E-04  1.0000E+00 -4.4035E-12 REF_ELEC
NA             8.5554E-02  1.5360E-03  1.5537E-50 -2.8431E+05 SER
CL             8.5554E-02  1.5360E-03  1.2078E-30 -1.7077E+05 SER
FE             1.5041E-02  2.7005E-04  5.2232E-26 -1.4431E+05 SER
CR             1.9232E-03  3.4530E-05  1.2572E-53 -3.0196E+05 SER
NI             8.5193E-04  1.5296E-05  1.0073E-15 -8.5603E+04 SER
CO             1.6968E-04  3.0465E-06  1.5331E-20 -1.1310E+05 SER

AQUEOUS      Status      Driving force  0.0000E+00
Moles 5.5653E+01, Mass 1.0045E+03, Volume fraction 1.0000E+00 Mole fractions:
H2O 9.96925E-01 ZE 4.72606E-07 FE 1.08577E-11
NA 1.53727E-03 NI 2.36161E-07 CR 2.55062E-13
CL 1.53727E-03 CO 1.31447E-10 H+1 -2.25543E-10
Constitution:  SiteFraction  Molality  Activity  log10Act
H2O           9.96925E-01  5.55084E+01  9.96603E-01 -0.0015
NA+1          1.53727E-03  8.55948E-02  6.73703E-02 -1.1715
CL-1          1.53727E-03  8.55948E-02  6.73703E-02 -1.1715
NI+2          2.35950E-07  1.31376E-05  5.07139E-06 -5.2949
OH-1          2.28889E-09  1.27444E-07  1.00279E-07 -6.9988
H+1           2.27916E-09  1.26903E-07  1.00000E-07 -7.0000
NIOH+1        2.10599E-10  1.17261E-08  9.23842E-09 -8.0344
CO+2          1.31447E-10  7.31890E-09  2.82496E-09 -8.5490
FE+2          6.13590E-12  3.41645E-10  1.31278E-10 -9.8818
FEOH+1        4.72178E-12  2.62907E-10  2.07132E-10 -9.6838
CRO+1         2.23303E-13  1.24334E-11  9.79571E-12 -11.0090
CROH+2        2.36100E-14  1.31459E-12  5.06585E-13 -12.2953
HCRO2         8.03267E-15  4.47256E-13  4.47228E-13 -12.3495
CR+3          7.04094E-17  3.92037E-15  4.60120E-16 -15.3371
CRO2-1        4.58077E-17  2.55056E-15  2.00946E-15 -14.6969
H2            1.06307E-19  5.91913E-18  5.91876E-18 -17.2278
FEOH+2        4.31923E-20  2.40493E-18  9.26752E-19 -18.0330
O2            1.00000E-20  5.56796E-19  2.17223E-58 -57.6631
FEO3H3-1      1.00000E-20  5.56796E-19  1.76819E-51 -50.7525
FECL+2        1.00000E-20  5.56796E-19  2.94449E-23 -22.5310
FE2O2H2+4     1.00000E-20  5.56796E-19  3.71178E-35 -34.4304
FE+3          1.00000E-20  5.56796E-19  1.53750E-23 -22.8132
H2O           1.00000E-20  5.56796E-19  3.35574E-46 -45.4742
HClO          1.00000E-20  5.56796E-19  2.84935E-45 -44.5453
CRO4-2        1.00000E-20  5.56796E-19  1.26903E-34 -33.8965
HClO2         1.00000E-20  5.56796E-19  1.02675E-87 -86.9885
HCRO4-1       1.00000E-20  5.56796E-19  3.83517E-35 -34.4162

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CR2O7-2      1.00000E-20  5.56796E-19  5.34416E-68  -67.2721
HO2-1        1.00000E-20  5.56796E-19  7.10153E-51  -50.1486
CR+2         1.00000E-20  5.56796E-19  2.20654E-23  -22.6563
CO1H2O2      1.00000E-20  5.56796E-19  2.7988E-105  -104.5530
CO+3         1.00000E-20  5.56796E-19  3.73219E-42  -41.4280
O3           1.00000E-20  5.56796E-19  2.0474E-113  -112.6888
CLO4-1       1.00000E-20  5.56796E-19  5.5717E-133  -132.2540
CLO3-1       1.00000E-20  5.56796E-19  1.0705E-105  -104.9704
CLO2-1       1.00000E-20  5.56796E-19  1.07460E-82  -81.9688
CLO2         1.00000E-20  5.56796E-19  1.1652E-100  -99.9336
CLO-1        1.00000E-20  5.56796E-19  6.17706E-46  -45.2092
CL2          1.00000E-20  5.56796E-19  4.04170E-50  -49.3934
Solution Properties:  pH = 7.0000  Eh = -0.0000 V  I = 0.0856
                    pe = -0.0000  Ah = -0.0000 kJ  m* = 0.1712
                    Aw = 0.9966  Os = 1.1033  pKw = 13.9973
                    At1= 1.0000E-20  At2= 1.2744E-07 (equiv_mol/kg_H2O)

HEMATITE      Status ENTERED  Driving force 0.0000E+00
Moles 3.3409E-02, Mass 1.0670E+00, Volume fraction 0.0000E+00  Mole fractions:
ZE 1.20000E+00 NI 0.00000E+00 NA 0.00000E+00
H2O 6.00000E-01 CR 0.00000E+00 CO 0.00000E+00
FE 4.00000E-01 CL 0.00000E+00 H+1 -1.20000E+00

NIFE2O4       Status ENTERED  Driving force 0.0000E+00
Moles 5.8715E-03, Mass 1.9660E-01, Volume fraction 0.0000E+00  Mole fractions:
ZE 1.14286E+00 NI 1.42857E-01 NA 0.00000E+00
H2O 5.71429E-01 CR 0.00000E+00 CO 0.00000E+00
FE 2.85714E-01 CL 0.00000E+00 H+1 -1.14286E+00

CR2O3         Status ENTERED  Driving force 0.0000E+00
Moles 3.9597E-03, Mass 1.2037E-01, Volume fraction 0.0000E+00  Mole fractions:
ZE 1.20000E+00 NI 0.00000E+00 NA 0.00000E+00
H2O 6.00000E-01 FE 0.00000E+00 CO 0.00000E+00
CR 4.00000E-01 CL 0.00000E+00 H+1 -1.20000E+00

COCR2O4       Status ENTERED  Driving force 0.0000E+00
Moles 1.1877E-03, Mass 3.8504E-02, Volume fraction 0.0000E+00  Mole fractions:
ZE 1.14286E+00 CO 1.42857E-01 NA 0.00000E+00
H2O 5.71429E-01 NI 0.00000E+00 FE 0.00000E+00
CR 2.85714E-01 CL 0.00000E+00 H+1 -1.14286E+00
POLY_3: l-st p
... the command in full is LIST_STATUS
*** STATUS FOR ALL PHASES
PHASE          STATUS          DRIVING FORCE          MOLES
NIFE2O4        ENTERED          0.000000E+00          5.871536E-03
HEMATITE        ENTERED          0.000000E+00          3.340878E-02
CR2O3          ENTERED          0.000000E+00          3.959678E-03
COCR2O4        ENTERED          0.000000E+00          1.187738E-03
AQUEOUS        ENTERED          0.000000E+00          5.565313E+01
FE2O3          ENTERED          -1.007600E-01          0.000000E+00
FE2O2O2H2      ENTERED          -1.872978E-01          0.000000E+00
FEOOH          ENTERED          -2.260402E-01          0.000000E+00
COFE2O4        ENTERED          -8.149192E-01          0.000000E+00
FEO3H3         ENTERED          -1.157510E+00          0.000000E+00
NICR2O4        ENTERED          -1.415362E+00          0.000000E+00
FE2O3_GAMMA    ENTERED          -1.461433E+00          0.000000E+00
MAGNETITE      ENTERED          -1.556302E+00          0.000000E+00
NIO2H2         ENTERED          -3.146330E+00          0.000000E+00
NIO            ENTERED          -4.159999E+00          0.000000E+00
ENTERED PHASES WITH DRIVING FORCE LESS THAN -4.169527E+00
NIO_S2 HALITE COO2H2 FEO2H2 NA2CR2O4 NA2FEO2 CO3O4 WUSTITE COO CRO2 NA2CRO4
NA2CRO4_S2 NIOOH CR5O12 NAOH NAOH_S2 CR8O21 CRO3 GAS NA2O2 NA2O2_S2 NA2O
NA2O_S2 NA2O_S3 NAO2 FCC_A1 BCC_A2
SUSPENDED PHASES:
REF ELECTRODE
POLY_3: sh b n n(*)
... the command in full is SHOW_VALUE
B=1005.9467
N=55.697555
N(H2O)=55.508435, N(H+1)=-5.2909903E-2, N(ZE)=5.2936192E-2, N(NA)=8.5554E-2,
N(CL)=8.5554E-2, N(FE)=1.5041094E-2, N(CR)=1.9232249E-3,
N(NI)=8.5193389E-4, N(CO)=1.6968422E-4
POLY_3:
POLY_3: @@... Saving the workspace for the single-point equilibrium
POLY_3: @@ of the Fe-Cr-Ni-Co + H2O-NaCl system:
POLY_3: save TCEX53 c.POLY3 y
... the command in full is SAVE_WORKSPACES
POLY_3:Hit RETURN to continuePOLY_3:
POLY_3: @@ =====
POLY_3: @@ Step 4: Pourbaix Diagram Mapping for Fe-Cr-Ni-Co + H2O-NaCl system
POLY_3: @@ *****
POLY_3:
POLY_3: @@... Defining the mapping variables for Pourbaix-diagram mapping:
POLY_3: @@ pH from 0 to 14
POLY_3: @@ Eh from -1.2 to 1.5 (V)
POLY_3: s-a-v 1 lnacr(H+1) -32.22994 0 0.5
... the command in full is SET_AXIS_VARIABLE
POLY_3: s-a-v 2 mur(Ze) -150000 200000 5000
... the command in full is SET_AXIS_VARIABLE
POLY_3: l-a-v
... the command in full is LIST_AXIS_VARIABLE
Axis No 1: LNACR(H+1) Min: -32.22994 Max: 0 Inc: 0.5
Axis No 2: MUR(ZE) Min: -150000 Max: 200000 Inc: 5000
POLY_3:
POLY_3: @@... Adding the starting points as initial equilibria:
POLY_3: @@ (they may be enforced in 2 or 4 directions with the option >)
POLY_3: @@
POLY_3: add 1>
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add -1>
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add 2>
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3: add -2>
... the command in full is ADD_INITIAL_EQUILIBRIUM
POLY_3:
POLY_3: @@... One may have more starting points at other pH-Eh conditions
POLY_3: @@ [corresponding to varied lnacr(H+1) and mur(Ze) values],
POLY_3: @@ and add them as initial equilibria.
POLY_3: @@
POLY_3: @@ s-c lnacr(H+1)=-23.0
POLY_3: @@ s-c mur(ZE)=-2000
POLY_3: @@ l-c

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POLY_3: @@ c-e
POLY_3: @@ l-e ,x
POLY_3: @@
POLY_3:
POLY_3:
POLY_3: li-in-eq
... the command in full is LIST INITIAL EQUILIBRIA
No 1 +1> P=100000, T=298.15, B(H2O)=1000., N(NA)=8.5554E-2, N(CL)=8.5554E-2,
N(FE)=1.5041094E-2, N(CR)=1.9232249E-3, N(NI)=8.5193389E-4,
N(CO)=1.6968422E-4, LNACR(H+1)=-16.118096, MUR(ZE)=-4.4035374E-12
No 2 -1> P=100000, T=298.15, B(H2O)=1000., N(NA)=8.5554E-2, N(CL)=8.5554E-2,
N(FE)=1.5041094E-2, N(CR)=1.9232249E-3, N(NI)=8.5193389E-4,
N(CO)=1.6968422E-4, LNACR(H+1)=-16.118096, MUR(ZE)=-4.4035374E-12
No 3 +2> P=100000, T=298.15, B(H2O)=1000., N(NA)=8.5554E-2, N(CL)=8.5554E-2,
N(FE)=1.5041094E-2, N(CR)=1.9232249E-3, N(NI)=8.5193389E-4,
N(CO)=1.6968422E-4, LNACR(H+1)=-16.118096, MUR(ZE)=-4.4035374E-12
No 4 -2> P=100000, T=298.15, B(H2O)=1000., N(NA)=8.5554E-2, N(CL)=8.5554E-2,
N(FE)=1.5041094E-2, N(CR)=1.9232249E-3, N(NI)=8.5193389E-4,
N(CO)=1.6968422E-4, LNACR(H+1)=-16.118096, MUR(ZE)=-4.4035374E-12
POLY_3:
POLY_3: @@... Saving the workspace for the Pourbaix-diagram settings
POLY_3: @@ of the Fe-Cr-Ni-Co + H2O-NaCl system:
POLY_3: save TCEX53_d.POLY3 y
... the command in full is SAVE WORKSPACES
POLY_3:Hit RETURN to continuePOLY_3:
POLY_3: @@... Performing the mapping calculation:
POLY_3: @@
POLY_3: @@ Due to the complexity of aqueous solution model (SIT or HKF),
POLY_3: @@ a complete mapping calculation of the Pourbaix-diagram type
POLY_3: @@ may take a rather long time. Please be patient...
POLY_3: @@
POLY_3: MAP
Version S mapping is selected

Organizing start points

Using ADDED start equilibria

Tie-lines not in the plane of calculation

Generating start point 1
Generating start point 2
Generating start point 3
Generating start point 4
Generating start point 5
Generating start point 6
Generating start point 7
Generating start point 8
Generating start point 9
Generating start point 10
Working hard
Generating start point 11
Generating start point 12

Phase region boundary 1 at: -1.541E+01 -4.404E-12
AQUEOUS
COCR2O4
CR2O3
** FECR2O4
HEMATITE
NIFE2O4
Calculated.. 35 equilibria
Terminating at axis limit.

Phase region boundary 2 at: -3.223E+01 -4.165E+04
AQUEOUS
COCR2O4
CR2O3
** FECR2O4
HEMATITE
NIFE2O4
Calculated. 38 equilibria

Phase region boundary 3 at: -1.404E+01 3.415E+03
AQUEOUS
COCR2O4
CR2O3
** FECR2O4
HEMATITE
** NIFE2O4

Phase region boundary 4 at: -1.404E+01 3.415E+03
AQUEOUS
COCR2O4
CR2O3
** FECR2O4
HEMATITE
Calculated. 7 equilibria

Phase region boundary 5 at: -1.110E+01 1.070E+04
AQUEOUS
** COCR2O4
CR2O3
** FECR2O4
HEMATITE

Phase region boundary 6 at: -1.110E+01 1.070E+04
AQUEOUS
CR2O3
** FECR2O4
HEMATITE
Calculated. 8 equilibria

Phase region boundary 7 at: -7.729E+00 1.905E+04
AQUEOUS
CR2O3
** FECR2O4
** HEMATITE

Phase region boundary 8 at: -7.729E+00 1.905E+04
AQUEOUS
CR2O3
** FECR2O4
Calculated. 9 equilibria

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Phase region boundary 9 at: -7.729E+00 -1.955E+04
** GAS
  AQUEOUS
  CR2O3
** FECR2O4

Phase region boundary 10 at: -7.729E+00 -1.955E+04
  GAS
  AQUEOUS
  CR2O3
** FECR2O4
Calculated.                3 equilibria

Phase region boundary 11 at: -7.169E+00 -1.817E+04
  GAS
  AQUEOUS
** CR2O3
** FECR2O4

Phase region boundary 12 at: -7.169E+00 -1.817E+04
  GAS
  AQUEOUS
** FECR2O4
Calculated                44 equilibria

Phase region boundary 13 at: -7.169E+00 -1.817E+04
  GAS
  AQUEOUS
** CR2O3
Calculated.                2 equilibria

Phase region boundary 14 at: -7.259E+00 -1.839E+04
** GAS
  AQUEOUS
** CR2O3

Phase region boundary 15 at: -7.259E+00 -1.839E+04
  AQUEOUS
** CR2O3
Calculated.                10 equilibria

Phase region boundary 16 at: -7.259E+00  2.259E+04
  AQUEOUS
** CR2O3
** HEMATITE

Phase region boundary 17 at: -7.259E+00  2.259E+04
  AQUEOUS
** CR2O3
  HEMATITE
Calculated.                32 equilibria

Phase region boundary 18 at: -1.110E+01  7.654E+04
  AQUEOUS
** COCR2O4
** CR2O3
  HEMATITE

Phase region boundary 19 at: -1.110E+01  7.654E+04
  AQUEOUS
  COCR2O4
** CR2O3
  HEMATITE
Calculated.                7 equilibria

Phase region boundary 20 at: -1.404E+01  6.628E+04
  AQUEOUS
  COCR2O4
** CR2O3
  HEMATITE
** NIFE2O4

Phase region boundary 21 at: -1.404E+01  6.628E+04
  AQUEOUS
  COCR2O4
** CR2O3
  HEMATITE
  NIFE2O4
Calculated..                38 equilibria
Terminating at axis limit.

Phase region boundary 22 at: -1.404E+01  6.628E+04
  AQUEOUS
  COCR2O4
  HEMATITE
** NIFE2O4
Calculated.                1 equilibria

Phase region boundary 23 at: -1.404E+01  6.733E+04
  AQUEOUS
** CO3O4
  COCR2O4
  HEMATITE
** NIFE2O4

Phase region boundary 24 at: -1.404E+01  6.733E+04
  AQUEOUS
  CO3O4
  COCR2O4
  HEMATITE
** NIFE2O4
Calculated.                2 equilibria

Phase region boundary 25 at: -1.404E+01  6.745E+04
  AQUEOUS
  CO3O4
** COCR2O4
  HEMATITE
** NIFE2O4

Phase region boundary 26 at: -1.404E+01  6.745E+04
  AQUEOUS
  CO3O4
  HEMATITE
** NIFE2O4
Calculated.                5 equilibria

```

```

Phase region boundary 27 at: -1.404E+01 8.332E+04
** GAS
  AQUEOUS
  CO3O4
  HEMATITE
** NIFE2O4

Phase region boundary 28 at: -1.404E+01 8.332E+04
  GAS
  AQUEOUS
  CO3O4
  HEMATITE
** NIFE2O4
Calculated.                11 equilibria

Phase region boundary 29 at: -1.257E+01 8.794E+04
  GAS
  AQUEOUS
  CO3O4
** HALITE
  HEMATITE
** NIFE2O4

Phase region boundary 30 at: -1.257E+01 8.794E+04
  GAS
  AQUEOUS
  CO3O4
  HALITE
  HEMATITE
** NIFE2O4
Calculated                33 equilibria

Phase region boundary 31 at: -1.257E+01 8.794E+04
  GAS
  AQUEOUS
  CO3O4
** HALITE
  HEMATITE
Calculated.                9 equilibria

Phase region boundary 32 at: -8.749E+00 9.740E+04
  GAS
  AQUEOUS
** CO3O4
** HALITE
  HEMATITE

Phase region boundary 33 at: -8.749E+00 9.740E+04
  GAS
  AQUEOUS
** HALITE
  HEMATITE
Calculated.                18 equilibria

Phase region boundary 34 at: -1.463E+00 1.159E+05
  GAS
  AQUEOUS
** HALITE
** HEMATITE

Phase region boundary 35 at: -1.463E+00 1.159E+05
  GAS
  AQUEOUS
** HALITE
Calculated                52 equilibria

Phase region boundary 36 at: -1.463E+00 1.159E+05
  GAS
  AQUEOUS
** HEMATITE
Calculated                5 equilibria

Phase region boundary 37 at: -1.463E+00 1.159E+05
  GAS
  AQUEOUS
  HALITE
** HEMATITE
Calculated                27 equilibria

Phase region boundary 38 at: -8.749E+00 9.740E+04
  GAS
  AQUEOUS
** CO3O4
  HEMATITE
Calculated.                8 equilibria

Phase region boundary 39 at: -1.021E+01 9.281E+04
** GAS
  AQUEOUS
** CO3O4
  HEMATITE

Phase region boundary 40 at: -1.021E+01 9.281E+04
  AQUEOUS
** CO3O4
  HEMATITE
Calculated.                5 equilibria

Phase region boundary 41 at: -1.211E+01 7.398E+04
  AQUEOUS
** CO3O4
** COCR2O4
  HEMATITE

Phase region boundary 42 at: -1.211E+01 7.398E+04
  AQUEOUS
** CO3O4
  COCR2O4
  HEMATITE
Calculated.                5 equilibria
Terminating at known equilibrium

Phase region boundary 43 at: -1.211E+01 7.398E+04
  AQUEOUS
** COCR2O4

```

HEMATITE  
Calculated. 4 equilibria  
Terminating at known equilibrium

Phase region boundary 44 at: -1.211E+01 7.398E+04  
AQUEOUS  
CO3O4  
\*\* COCR2O4  
HEMATITE  
Calculated. 5 equilibria  
Terminating at known equilibrium

Phase region boundary 45 at: -1.021E+01 9.281E+04  
\*\* GAS  
AQUEOUS  
HEMATITE  
Calculated. 20 equilibria

Phase region boundary 46 at: -1.208E+00 1.151E+05  
\*\* GAS  
AQUEOUS  
\*\* HEMATITE

Phase region boundary 47 at: -1.208E+00 1.151E+05  
\*\* GAS  
AQUEOUS  
Calculated.. 4 equilibria  
Terminating at axis limit.

Phase region boundary 48 at: -1.208E+00 1.151E+05  
AQUEOUS  
\*\* HEMATITE  
Calculated. 28 equilibria  
Terminating at known equilibrium

Phase region boundary 49 at: -1.208E+00 1.151E+05  
GAS  
AQUEOUS  
\*\* HEMATITE  
Calculated 24 equilibria

Phase region boundary 50 at: -1.021E+01 9.281E+04  
\*\* GAS  
AQUEOUS  
CO3O4  
HEMATITE  
Calculated. 9 equilibria  
Terminating at known equilibrium

Phase region boundary 51 at: -8.749E+00 9.740E+04  
GAS  
AQUEOUS  
\*\* CO3O4  
HALITE  
HEMATITE  
Calculated 39 equilibria

Phase region boundary 52 at: -1.257E+01 8.794E+04  
GAS  
AQUEOUS  
CO3O4  
\*\* HALITE  
HEMATITE  
NIFE2O4  
Calculated.. 41 equilibria  
Terminating at axis limit.

Phase region boundary 53 at: -1.404E+01 8.332E+04  
\*\* GAS  
AQUEOUS  
CO3O4  
HEMATITE  
NIFE2O4  
Calculated.. 38 equilibria  
Terminating at axis limit.

Phase region boundary 54 at: -1.404E+01 6.745E+04  
AQUEOUS  
CO3O4  
\*\* COCR2O4  
HEMATITE  
NIFE2O4  
Calculated. 27 equilibria

Phase region boundary 55 at: -2.249E+01 3.456E+04  
AQUEOUS  
CO3O4  
\*\* COCR2O4  
\*\* COFE2O4  
HEMATITE  
NIFE2O4

Phase region boundary 56 at: -2.249E+01 3.456E+04  
AQUEOUS  
CO3O4  
\*\* COCR2O4  
COFE2O4  
HEMATITE  
NIFE2O4

+++++

Phase region boundary 57 at: -2.249E+01 3.456E+04  
AQUEOUS  
CO3O4  
\*\* COFE2O4  
HEMATITE  
NIFE2O4  
Calculated.. 21 equilibria  
Terminating at axis limit.

Phase region boundary 58 at: -2.249E+01 3.456E+04  
AQUEOUS  
CO3O4  
COCR2O4  
\*\* COFE2O4

```

HEMATITE
NIFE204
Calculated.                2  equilibria

Phase region boundary  59 at: -2.239E+01  3.480E+04
AQUEOUS
** CO3O4
COCR204
** COFE204
HEMATITE
NIFE204

Phase region boundary  60 at: -2.239E+01  3.480E+04
AQUEOUS
COCR204
** COFE204
HEMATITE
NIFE204
Calculated..                21  equilibria
Terminating at axis limit.

Phase region boundary  61 at: -2.239E+01  3.480E+04
AQUEOUS
** CO3O4
COCR204
HEMATITE
NIFE204
Calculated.                18  equilibria
Terminating at known equilibrium

Phase region boundary  62 at: -2.239E+01  3.480E+04
AQUEOUS
** CO3O4
COCR204
COFE204
HEMATITE
NIFE204
Calculated.                2  equilibria
Terminating at known equilibrium

Phase region boundary  63 at: -1.404E+01  6.628E+04
AQUEOUS
COCR204
CR2O3
HEMATITE
** NIFE204
Calculated.                14  equilibria
Terminating at known equilibrium

Phase region boundary  64 at: -1.110E+01  7.654E+04
AQUEOUS
** COCR204
CR2O3
HEMATITE
Calculated.                15  equilibria
Terminating at known equilibrium

Phase region boundary  65 at: -7.259E+00  2.259E+04
AQUEOUS
CR2O3
** HEMATITE
Calculated.                2  equilibria
Terminating at known equilibrium

Phase region boundary  66 at: -7.259E+00 -1.839E+04
** GAS
AQUEOUS
Calculated..                16  equilibria
Terminating at axis limit.

Phase region boundary  67 at: -7.259E+00 -1.839E+04
** GAS
AQUEOUS
CR2O3
Calculated.                2  equilibria
Terminating at known equilibrium

Phase region boundary  68 at: -7.169E+00 -1.817E+04
GAS
AQUEOUS
** CR2O3
FECCR204
Calculated.                3  equilibria

Phase region boundary  69 at: -7.752E+00 -1.961E+04
** GAS
AQUEOUS
** CR2O3
FECCR204

Phase region boundary  70 at: -7.752E+00 -1.961E+04
AQUEOUS
** CR2O3
FECCR204
Calculated.                9  equilibria

Phase region boundary  71 at: -7.752E+00  1.899E+04
AQUEOUS
** CR2O3
FECCR204
** HEMATITE

Phase region boundary  72 at: -7.752E+00  1.899E+04
AQUEOUS
** CR2O3
FECCR204
HEMATITE
Calculated.                8  equilibria
Terminating at known equilibrium

Phase region boundary  73 at: -7.752E+00  1.899E+04
AQUEOUS
FECCR204
** HEMATITE
Calculated.                16  equilibria

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Phase region boundary 74 at: -1.286E+01 -1.893E+04  
 AQUEOUS  
 FECR2O4  
 \*\* HEMATITE  
 \*\* MAGNETITE

Phase region boundary 75 at: -1.286E+01 -1.893E+04  
 AQUEOUS  
 FECR2O4  
 \*\* HEMATITE  
 MAGNETITE  
 Calculated. 4 equilibria

Phase region boundary 76 at: -1.395E+01 -2.164E+04  
 AQUEOUS  
 \*\* COFE2O4  
 FECR2O4  
 \*\* HEMATITE  
 MAGNETITE

Phase region boundary 77 at: -1.395E+01 -2.164E+04  
 AQUEOUS  
 COFE2O4  
 FECR2O4  
 \*\* HEMATITE  
 MAGNETITE  
 Calculated. 2 equilibria

Phase region boundary 78 at: -1.404E+01 -2.186E+04  
 AQUEOUS  
 COFE2O4  
 FECR2O4  
 \*\* HEMATITE  
 MAGNETITE  
 \*\* NIFE2O4

Phase region boundary 79 at: -1.404E+01 -2.186E+04  
 AQUEOUS  
 COFE2O4  
 FECR2O4  
 \*\* HEMATITE  
 MAGNETITE  
 NIFE2O4  
 Calculated.. 38 equilibria  
 Terminating at axis limit.

Phase region boundary 80 at: -1.404E+01 -2.186E+04  
 AQUEOUS  
 COFE2O4  
 FECR2O4  
 MAGNETITE  
 \*\* NIFE2O4  
 Calculated. 5 equilibria

Phase region boundary 81 at: -1.555E+01 -3.682E+04  
 AQUEOUS  
 \*\* BCC\_A2  
 COFE2O4  
 FECR2O4  
 MAGNETITE  
 \*\* NIFE2O4

Phase region boundary 82 at: -1.555E+01 -3.682E+04  
 AQUEOUS  
 BCC\_A2  
 COFE2O4  
 FECR2O4  
 MAGNETITE  
 \*\* NIFE2O4  
 Calculated.. 35 equilibria  
 Terminating at axis limit.

Phase region boundary 83 at: -1.555E+01 -3.682E+04  
 AQUEOUS  
 \*\* BCC\_A2  
 COFE2O4  
 FECR2O4  
 MAGNETITE  
 Calculated. 2 equilibria

Phase region boundary 84 at: -1.548E+01 -3.681E+04  
 AQUEOUS  
 \*\* BCC\_A2  
 \*\* COFE2O4  
 FECR2O4  
 MAGNETITE

Phase region boundary 85 at: -1.548E+01 -3.681E+04  
 AQUEOUS  
 \*\* BCC\_A2  
 FECR2O4  
 MAGNETITE  
 Calculated. 4 equilibria

Phase region boundary 86 at: -1.473E+01 -3.690E+04  
 \*\* GAS  
 AQUEOUS  
 \*\* BCC\_A2  
 FECR2O4  
 MAGNETITE

Phase region boundary 87 at: -1.473E+01 -3.690E+04  
 GAS  
 AQUEOUS  
 \*\* BCC\_A2  
 FECR2O4  
 MAGNETITE  
 Calculated. 7 equilibria

Phase region boundary 88 at: -1.390E+01 -3.486E+04  
 GAS  
 AQUEOUS  
 \*\* BCC\_A2  
 FECR2O4  
 \*\* MAGNETITE



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Phase region boundary 89 at: -1.390E+01 -3.486E+04
  GAS
  AQUEOUS
  ** BCC_A2
  FECD204
Calculated.                8 equilibria

Phase region boundary 90 at: -1.280E+01 -3.214E+04
  GAS
  AQUEOUS
  ** BCC_A2
  FECD204
  ** HALITE

Phase region boundary 91 at: -1.280E+01 -3.214E+04
  GAS
  AQUEOUS
  ** BCC_A2
  FECD204
  HALITE
Calculated                201 equilibria

Phase region boundary 92 at: -1.280E+01 -3.214E+04
  GAS
  AQUEOUS
  FECD204
  ** HALITE
Calculated.                14 equilibria

Phase region boundary 93 at: -7.005E+00 -1.778E+04
  GAS
  AQUEOUS
  ** FECD204
  ** 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
  ** FECD204

+

Phase region boundary 96 at: -7.005E+00 -1.778E+04
  GAS
  AQUEOUS
  ** FECD204
  HALITE
Calculated                62 equilibria

Phase region boundary 97 at: -1.280E+01 -3.214E+04
  GAS
  AQUEOUS
  BCC_A2
  FECD204
  ** HALITE
Calculated.                6 equilibria

Phase region boundary 98 at: -1.381E+01 -3.464E+04
  GAS
  AQUEOUS
  BCC_A2
  FECD204
  ** HALITE
  ** MAGNETITE

Phase region boundary 99 at: -1.381E+01 -3.464E+04
  GAS
  AQUEOUS
  BCC_A2
  FECD204
  ** HALITE
  MAGNETITE
Calculated..                38 equilibria
Terminating at axis limit.

Phase region boundary 100 at: -1.381E+01 -3.464E+04
  GAS
  AQUEOUS
  BCC_A2
  FECD204
  ** MAGNETITE

+

Phase region boundary 101 at: -1.381E+01 -3.464E+04
  GAS
  AQUEOUS
  BCC_A2
  FECD204
  HALITE
  ** MAGNETITE
Calculated                61 equilibria

Phase region boundary 102 at: -1.390E+01 -3.486E+04
  GAS
  AQUEOUS
  FECD204
  ** MAGNETITE
Calculated.                3 equilibria

Phase region boundary 103 at: -1.472E+01 -3.688E+04
  ** GAS
  AQUEOUS
  FECD204
  ** MAGNETITE

Phase region boundary 104 at: -1.472E+01 -3.688E+04
  AQUEOUS
  FECD204

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** MAGNETITE
Calculated.          5 equilibria
Terminating at known equilibrium

Phase region boundary 105 at: -1.472E+01 -3.688E+04
** GAS
  AQUEOUS
  FECR204
Calculated.          15 equilibria
Terminating at known equilibrium

Phase region boundary 106 at: -1.472E+01 -3.688E+04
** GAS
  AQUEOUS
  FECR204
  MAGNETITE
Calculated.          2 equilibria
Terminating at known equilibrium

Phase region boundary 107 at: -1.390E+01 -3.486E+04
  GAS
  AQUEOUS
  BCC_A2
  FECR204
** MAGNETITE
Calculated.          46 equilibria

Phase region boundary 108 at: -1.473E+01 -3.690E+04
** GAS
  AQUEOUS
  BCC_A2
  FECR204
  MAGNETITE
Calculated..          38 equilibria
Terminating at axis limit.

Phase region boundary 109 at: -1.548E+01 -3.681E+04
  AQUEOUS
** COFE204
  FECR204
  MAGNETITE
Calculated.          5 equilibria
Terminating at known equilibrium

Phase region boundary 110 at: -1.548E+01 -3.681E+04
  AQUEOUS
  BCC_A2
** COFE204
  FECR204
  MAGNETITE
Calculated..          37 equilibria
Terminating at axis limit.

Phase region boundary 111 at: -1.555E+01 -3.682E+04
  AQUEOUS
** BCC_A2
  COFE204
  FECR204
  MAGNETITE
  NIFE204
Calculated..          35 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 112 at: -1.404E+01 -2.186E+04
  AQUEOUS
  COFE204
  FECR204
  HEMATITE
  MAGNETITE
** NIFE204
Calculated.          1 equilibria

Phase region boundary 113 at: -1.404E+01 -2.186E+04
  AQUEOUS
  COFE204
  FECR204
  HEMATITE
** MAGNETITE
** NIFE204

Phase region boundary 114 at: -1.404E+01 -2.186E+04
  AQUEOUS
  COFE204
  FECR204
  HEMATITE
** NIFE204
Calculated.          4 equilibria

Phase region boundary 115 at: -1.404E+01 -1.073E+04
  AQUEOUS
** COCR204
  COFE204
  FECR204
  HEMATITE
** NIFE204

Phase region boundary 116 at: -1.404E+01 -1.073E+04
  AQUEOUS
  COCR204
  COFE204
  FECR204
  HEMATITE
** NIFE204
Calculated.          1 equilibria
Terminating at known equilibrium

Phase region boundary 117 at: -1.404E+01 -1.073E+04
  AQUEOUS
** COCR204
  COFE204
  FECR204
  HEMATITE
Calculated.          2 equilibria

Phase region boundary 118 at: -1.395E+01 -1.051E+04

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    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

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Calculated.                1 equilibria
Terminating at known equilibrium

Phase region boundary 132 at: -1.541E+01 -4.404E-12
  AQUEOUS
  COCR2O4
  CR2O3
  ** FECR2O4
  HEMATITE
  NIFE2O4
Calculated.                4 equilibria
Terminating at known equilibrium

Phase region boundary 133 at: -3.020E+01 -4.404E-12
  AQUEOUS
  COCR2O4
  ** CR2O3
  HEMATITE
  NIFE2O4
Calculated..              9 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 134 at: -3.020E+01 -4.404E-12
  AQUEOUS
  COCR2O4
  ** CR2O3
  HEMATITE
  NIFE2O4
Calculated.              54 equilibria
Terminating at known equilibrium

Phase region boundary 135 at: -1.610E+01  5.964E+04
  AQUEOUS
  ** CO3O4
  COCR2O4
  HEMATITE
  NIFE2O4
Calculated.              21 equilibria
Terminating at known equilibrium

Phase region boundary 136 at: -1.610E+01  5.964E+04
  AQUEOUS
  ** CO3O4
  COCR2O4
  HEMATITE
  NIFE2O4
Calculated.              7 equilibria
Terminating at known equilibrium

Phase region boundary 137 at: -1.612E+01  5.959E+04
  AQUEOUS
  ** CO3O4
  COCR2O4
  HEMATITE
  NIFE2O4
Calculated.              14 equilibria
Terminating at known equilibrium

Phase region boundary 138 at: -1.612E+01  5.959E+04
  AQUEOUS
  ** CO3O4
  COCR2O4
  HEMATITE
  NIFE2O4
Calculated.              6 equilibria
Terminating at known equilibrium

Phase region boundary 139 at: -1.612E+01  5.825E+04
  AQUEOUS
  COCR2O4
  ** CR2O3
  HEMATITE
  NIFE2O4
Calculated..             34 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 140 at: -1.612E+01  5.825E+04
  AQUEOUS
  COCR2O4
  ** CR2O3
  HEMATITE
  NIFE2O4
Calculated.              6 equilibria
Terminating at known equilibrium

Phase region boundary 141 at: -1.612E+01 -1.748E+03
  AQUEOUS
  COCR2O4
  CR2O3
  ** FECR2O4
  HEMATITE
  NIFE2O4
Calculated..             34 equilibria
Terminating at known equilibrium
Terminating at axis limit.

Phase region boundary 142 at: -1.612E+01 -1.748E+03
  AQUEOUS
  COCR2O4
  CR2O3
  ** FECR2O4
  HEMATITE
  NIFE2O4
Calculated.              6 equilibria
Terminating at known equilibrium
*** BUFFER SAVED ON FILE:
c:\jenkins\workspace\Thermo-Calc-Generate-Console-Examples\examples\tcex53\TCEX
53_d.POLY3
CPU time for mapping                926 seconds
POLY_3:
POLY_3: @@... Plotting the calculated Pourbaix diagram (& many others):
POLY_3: @@ -----
POLY_3: post

```

Setting automatic diagram axes

```

POST: l-sym
... the command in full is LIST_SYMBOLS
DEFINED CONSTANTS
  AH2O=55.508435, RNF=96485.309, ZERO=0
DEFINED FUNCTIONS AND VARIABLES%
  EH=MUR(ZE)/RNF
  PH=- LOG10(ACR(H+1,AQUEOUS)*AH2O )
  TEMP_C=T-273.15
POST:Hit RETURN to continuePOST:
POST: s-d-a x pH
... the command in full is SET_DIAGRAM_AXIS
POST: s-a-text x n pH
... the command in full is SET_AXIS_TEXT_STATUS
POST:

POST: s-d-a y Eh
... the command in full is SET_DIAGRAM_AXIS
POST: s-a-text y n Eh (V)
... the command in full is SET_AXIS_TEXT_STATUS
POST:

POST: s-t-m-s y
... the command in full is SET_TRUE_MANUAL_SCALING
COMMAND NOT SUPPORTED IN THIS PLOT DRIVER
POST: s-l-c e
... the command in full is SET_LABEL_CURVE_OPTION
POST:

POST: s-s-s x n 0 14
... the command in full is SET_SCALING_STATUS
POST: s-s-s y n -1.0 1.5
... the command in full is SET_SCALING_STATUS
POST: s-title Thermo-Calc Example 53-a
... the command in full is SET_TITLE
POST: pl,,,
... the command in full is PLOT_DIAGRAM

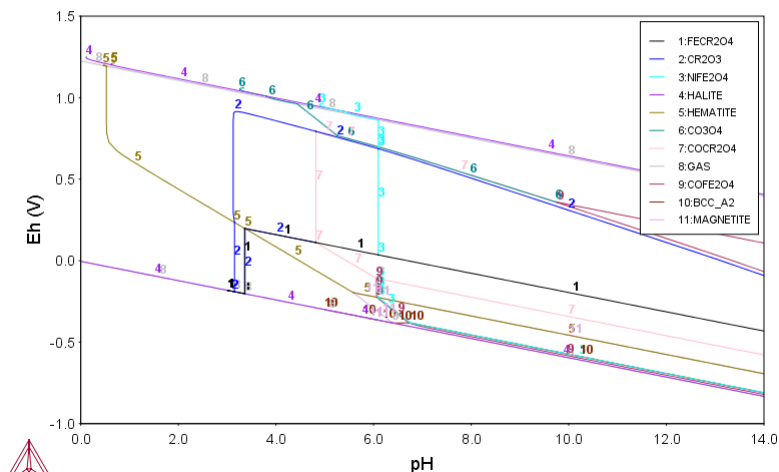
```

## Thermo-Calc Example 53-a

2016.05.16.15.21.17

PAQ2: H2O, H+1, ZE, NA, CL, FE, CR, NI, CO

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



```

POST: make TCEX53.EXP y
... the command in full is MAKE_EXPERIMENTAL_DATAFI
POST:Hit RETURN to continue
POST:

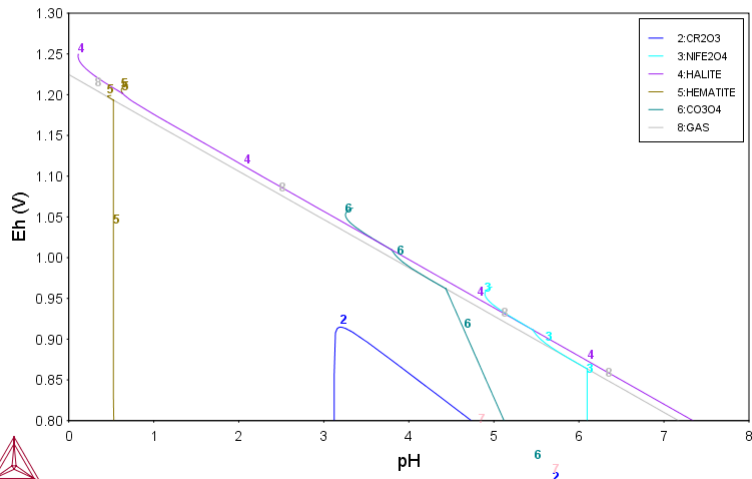
POST: s-s-s x n 0 8
... the command in full is SET_SCALING_STATUS
POST: s-s-s y n .8 1.3
... the command in full is SET_SCALING_STATUS
POST: s-title Thermo-Calc Example 53-b
... the command in full is SET_TITLE
POST:

POST: pl,,,
... the command in full is PLOT_DIAGRAM

```

### Thermo-Calc Example 53-b

2016.05.16.15.21.19  
 PAQ2: H2O, H+1, ZE, NA, CL, FE, CR, NI, CO  
 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



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

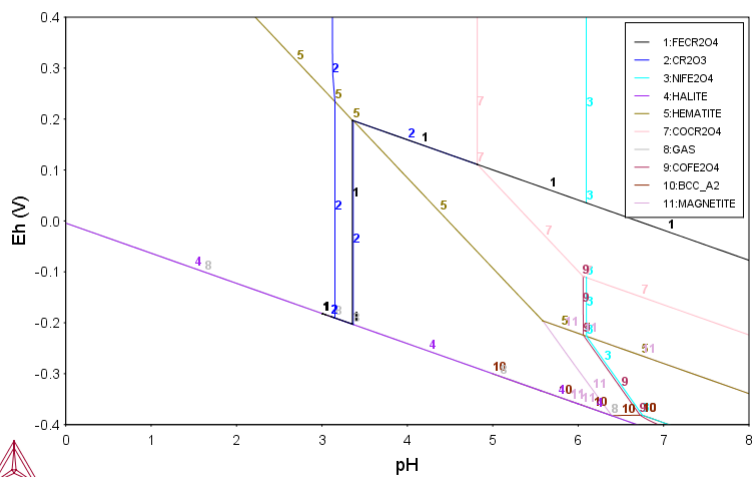
POST:

POST: pl,,,

... the command in full is PLOT DIAGRAM

### Thermo-Calc Example 53-c

2016.05.16.15.21.21  
 PAQ2: H2O, H+1, ZE, NA, CL, FE, CR, NI, CO  
 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



POST:Hit RETURN to continue

POST:

POST: @@

POST: @@ \*\*\*\*\*

POST: @@ From the same mapping calculations, one may plot many more diagrams,

POST: @@ using various X-Y axis variables (for such purposes, it is very

POST: @@ convenient to use pre-defined symbols as listed at the end of

POST: @@ this MACRO file).

POST: @@ \*\*\*\*\*

POST: @@

POST: SET-INTERACTIVE

... the command in full is SET\_INTERACTIVE\_MODE

POST:



# Pourbaix Diagrams

Educational Material





---

# Introduction to Pourbaix Diagrams

In this section:

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<i>About Pourbaix Diagrams in Thermo-Calc</i> .....	3
<i>Pourbaix Diagrams</i> .....	3
<i>Working with Pourbaix Diagrams</i> .....	5
<i>Key Concepts</i> .....	5
<i>Basic Settings and Definitions</i> .....	7

---

## About Pourbaix Diagrams in Thermo-Calc

This guide is for Thermo-Calc software users who know the basics of thermodynamics and want to know more about *Pourbaix Diagrams* below.

You are introduced to the concept of a Pourbaix diagram and shown how to interpret such diagrams through a series of examples.

Materials corrosion occurs almost everywhere. It may lead to serious material damages, unexpected application failures, tremendous economic costs and environmental degradations. Consequently, scientists and engineers must often conduct expensive and time-consuming corrosion experiments as part of failure analyses, risk evaluations, quality improvements and application enhancements.

Under certain conditions, when a metal or alloy is exposed to an aqueous solution with a concentration of inorganic/organic mixture, corrosion phenomena occur at a corresponding degree. During corrosion, some metallic phases dissolve, the metal or alloy surface gets damaged and some secondary solid phases form at the solid-liquid interfaces (such as oxides, hydroxides, silicates, sulphides, sulphates, carbonates, nitrates, phosphates, borates, or halides). Such corrosive chemical or electrochemical reactions can be studied by means of the so-called Pourbaix diagrams if the reactions reach their equilibrium states (Pourbaix, 1973, 1974; Cramer and Covino, 2003; Verink, 2011; Thompson et al., 2011).

## Pourbaix Diagrams

Marcel Pourbaix applied thermodynamics to predict materials corrosion resistance. He determined the phase stability relations in terms of varied pH and Eh values for an interaction system of metal and pure water or dilute aqueous solution. He presented the stability regions of metal and secondary phases (such as metal-oxides/hydroxides) on a pH-Eh diagram, which is now known as a Pourbaix diagram.

A Pourbaix diagram is a kind of phase diagram that shows the stability boundaries for a metal-aqueous interaction system. The phase boundaries are shown as a function of pH (acidity) and Eh (standard hydrogen electronic potential). An aqueous solution phase is always present in such a system. At a given pH and Eh, a metal may lose its stability to a soluble or corrosive aqueous solution, or be in equilibrium with either the aqueous solution (insoluble/immune) or with a secondary-phase file that has formed (consisting of oxides, hydroxides, sulphides or other solids). In the latter case, further dissolution of the passive or protective metal is prevented.

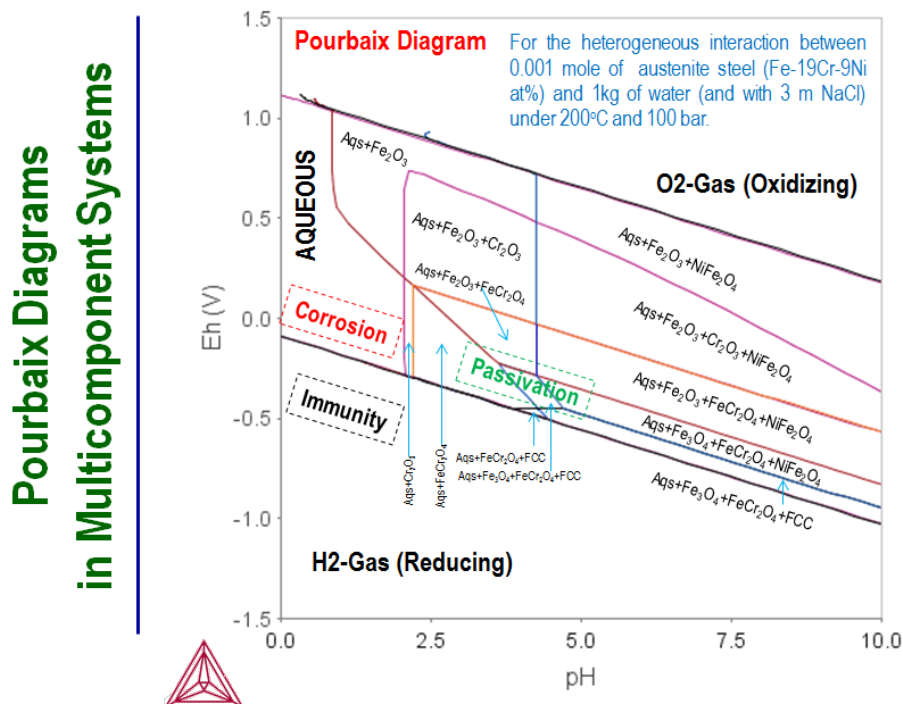
The speciation and partition in the aqueous solution and the interacting phases depend not only on pH and Eh, but also on other factors such as the bulk composition, temperature and pressure in the system. The interacting phases may be gas mixtures, stoichiometric solids or solid solutions.

A Pourbaix diagram is divided in regions of *immunity*, *corrosion* and *passivity*. These regions provides information about the stability of a particular metal or alloy in a specific aqueous electrochemical environment under certain pH, Eh, pressure and temperature conditions.

- The immunity region is the region in which there is no metal dissolution.
- The corrosion region is the region in which there is active metal dissolution.

- The passivation region is the region in which a protective metal-oxide film that prevents metal dissolution is formed.

The following shows these three regions in a Pourbaix diagram for the heterogeneous interaction between 0.001 mole of austenite steel (Fe-19Cr-9Ni [at%]) and 1 kg of water (with 3 m NaCl), at 200°C and 100 bar:



Depending on the system's bulk chemical composition, secondary phases may form during the transformation process. These can not only be oxides, but also be, for example, hydroxides, sulphides, sulphates, carbonates, nitrates, phosphates, borates, silicates, hydrous silicates and halides. Information about these secondary phases may help one understand the passivation behaviours in corrosion processes. For example, it may be important to understand whether any secondary phases are formed in different pH-Eh regions during hydrolysis, oxidation, reduction or other reaction processes.

In a Pourbaix diagram, the predominant ion boundaries are often represented by dashed and straight lines imposed on a traditional Pourbaix diagram for a simple interaction system (Pourbaix, 1973, 1974; Cramer and Covino, 2003; Verink, 2011; Thompson et al., 2011). Such a predominance boundary is normally an equal molality (or equal activity) line for a pair of two most-concentrated aqueous solute species (charged or neutral) involving a common metal. A line is then simply determined by a reaction constant of its corresponding electrochemical reaction in the homogeneous aqueous solution phase. However, this is not the case in Thermo-Calc.



You cannot get any information about predominant ion boundaries from a Pourbaix diagram in Thermo-Calc.

---

## Working with Pourbaix Diagrams

With the Thermo-Calc software package, Pourbaix diagrams can be calculated over a wide range of pressure, temperature and composition conditions for complex heterogeneous interactions between multicomponent primary alloy solution or compound phases, concentrated aqueous solutions (with dissolved inorganic and organic substances), complicated secondary solids and oxidizing/reducing gaseous mixtures. In the Console Mode, diagrams can be calculated and plotted either using the response-driven POURBAIX module or directly using the DATA, GIBBS, POLY and POST modules.

Note that it is possible in Thermo-Calc to set aqueous properties other than pH and Eh as axis variables. For example, the following properties can also be set as axis variables:  $A_h$  (electronic affinity),  $p_e$  (electronic activity  $\log_{10} A_{Cr}$ ),  $I_S$  (ionic strength),  $T_M$  (total aqueous concentration, in molality),  $O_C$  (Osmotic coefficient), activity or activity coefficient of solvent H<sub>2</sub>O, and activities or activity coefficients or concentrations in m (molality) of charged or neutral solute species.

Beside a concentrated aqueous solution phase handled by a proper thermodynamic model named SIT, HKF or PITZ, it is also possible to consider complex alloy solution phases or compound phases, as well as secondary solid phases and gaseous mixtures, which are treated by specific solution models.

Most frequently, a Pourbaix diagram is calculated for a specific alloyed phase with the initial alloying composition, such as the FCC solution phase in an austenite steel. However, it is possible to calculate a Pourbaix diagram for two co-existing phases, such as the FCC+BCC solution phases in a duplex steel for example, or even for more than two co-existing phases in a steel/alloy.

Note that each point on the lines in a pH-Eh diagram in Thermo-Calc represents a certain minimum state of Gibbs energy. When a line is crossed, a phase transformation should occur. This means that a Pourbaix diagram in Thermo-Calc does not provide any information about any predominant ion boundary.

## Key Concepts

The following are two key concepts important for understanding how aqueous solutions behave and how an aqueous-bearing heterogeneous interaction system is properly defined and calculated in Thermo-Calc.

### Effective Interaction Ratio

A pH-Eh plot is always related to a certain amount of initial alloys or other condensed materials that has effectively reacted with an aqueous solution in the system. This is the amount of condensed material that is fully in equilibrium with the defined aqueous solution phase. The amount is specified relative to an aqueous solution that is normally comprised of 1 kg of water with certain specified solute concentrations at certain temperature and pressure conditions. (This is why a calculated Pourbaix diagram is typically presented for an initial amount of the interacting metal or alloy at a certain level, such as 10<sup>-6</sup>, 1E-3, 0.1 or 1 mole of metal or alloy.) It is called the *Effective Interaction Ratio* (between the initial alloy or alloyed phases and the initial aqueous solution) and it is expressed in terms of molality (mol/kg).

The Effective Interaction Ratio is important for two reasons. First, the ratio has implications for kinetic or dynamic effects such as chemical reaction mechanism and kinetics, fluid flow dynamics, surface area and

interaction time. Secondly, the ratio, being expressed as  $10^{-6}$  mole of metal (or alloy), is the solubility limit that can be detected for cathodic corrosion protection by immunity.

One should always be careful when setting initial amounts and compositions in the original condensed materials, as well as when setting the initial concentrations of dissolved solutes in the original aqueous solution phase. It is often useful to make a series of calculations for different levels of initial amount of the interacting metal/alloy while the conditions are fixed for other settings (such as initial aqueous concentration, pressure, temperature, pH, and Eh).

## Solubility

When a heterogeneous equilibrium has a dissolving solution or mixture phase and a stoichiometric or solution phase, then the concept of solubility becomes important. A solubility of a phase (the solute) is its property of dissolving in the solvent phase. This concept concerns the constitution of a phase and is applied where one or several of the constituents are dominant (which is highly concentrated and dissolving) while there are only small amounts of the other remaining species (which are less concentrated and dissolved). The dissolving solution or mixture phase can be liquid, gas, aqueous or solid, as long as it has dissolving capacity. The stoichiometric or solution phase has some constituents which tend to be dissolved into the dissolving solution or mixture phase.

## Key Points about Solubility

- Under certain temperature, pressure and composition conditions, a Fe- or Cr-dominant BCC phase can dissolve certain amounts of Ni and C from a carbide phase such as M<sub>23</sub>C<sub>6</sub>, M<sub>7</sub>C<sub>3</sub> or M<sub>3</sub>C. The Ni and C elements in the carbides have the solubility defined relative to the BCC phase.
- An aqueous solution phase is always dominant in the solvent water, that is, H<sub>2</sub>O. Under specific temperature, pressure and aqueous composition conditions, any other element (such as Fe and C) or substance (such as a pure SO<sub>2</sub> gas, stoichiometric phase Cu<sub>2</sub>S and solution phase (Fe,Ni)<sub>1</sub>(O,Va)<sub>1</sub>) have a certain solubility limit in the defined aqueous solution.
- Under certain temperature and pressure conditions, and under given certain concentrations of other dissolved species in the mixture, an O<sub>2</sub>-dominant gaseous mixture phase can dissolve certain amounts of Fe<sup>+2</sup> or Fe<sup>+3</sup> species from magnetite (Fe<sub>3</sub>O<sub>4</sub>). The magnetite solid has solubility defined relative to the gaseous mixture under the given conditions.
- Under certain temperature and pressure condition, under specific concentrations of other dissolved species in the liquid phase, a Fe-dominant liquid mixture phase can dissolve certain amounts of, for example, Cr and O. The Cr and O components have the solubility defined in the liquid mixture.

## Basic Settings and Definitions

In a homogeneous aqueous solution or an aqueous-bearing heterogeneous interaction system, the most essential definition is for system-components there must be H<sub>2</sub>O, H<sup>+1</sup> and ZE (electron) plus those for elements dissolved in aqueous solution (such as Na, Cl, S) and associated in interacting metals/alloys (such as Fe, Cr, Mn, Mg, Ni, Al, Si, Zn). Three fundamental phases in a system are the AQUEOUS solution, the GAS mixture and the REF\_ELECTRODE. The REF\_ELECTRODE phase is used for setting the reference state for electrostatic potential in the system and for calculating the Eh condition (defined as  $MUR(ZE) / RNF$ ). Other phases should be appropriately selected and retrieved from critically-assessed databases that cover not only the target phases (solution or stoichiometric) in interacting metals/alloys but also the secondary phases (solution or stoichiometric). The two public databases PAQ and PAQS are specially designed as single-database choices that cover all kinds of phases necessary for calculations. However, these databases are each limited to a framework of a very small number of elements. When it comes to simulations of complex multicomponent systems with a wide variety of elements and phases, the thermodynamic data must be selected and retrieved from several databases: AQUEOUS solution and REF\_ELCTRODE phases must be retrieved from TCAQ or AQS; alloy phases (such as FCC\_A1, BCC\_A2, HCP\_A3, CEMENTITE) from alloy solution databases (such as SSOL for general alloy phases, TCFE for steel/Fe-alloy phases, TCAL for Al-based alloy phases; TCMG for Mg-based alloy phases, and TCNI for Ni-based superalloy phases); gaseous mixture phase and secondary phases from specific substance or solution databases (such as SSUB for GAS phase and various solid compound phases or TCOX for oxide solution phases). Note that the REF\_ELECTRODE phase should always be suspended in equilibrium

calculations, while GAS phase could be set as ENTERED, SUSPENDED or DORMANT, depending on the purpose of the calculation.

When defining an interaction system, the initial condition for the H<sub>2</sub>O component is always set as 1 kg of water. The initial composition conditions for dissolving and interacting elements are normally defined in moles (such as  $n(\text{Fe})=0.009$ ,  $n(\text{Cr})=5\text{E}-4$ ,  $n(\text{Ni})=3\text{E}-4$ ,  $n(\text{Mn})=5\text{E}-5$ ,  $n(\text{S})=5\text{E}-5$ ,  $n(\text{Na})=3$ ,  $n(\text{Cl})=3$ ). This makes it straightforward and convenient to count various related aqueous solution properties based on molality. The initial conditions for the H+1 and ZE components can be given as molar compositions (such as  $n(\text{H}+1)=0$ ,  $n(\text{ZE})=0$ ) or their activities or potentials (such as  $\ln \text{ACR}(\text{H}+1)=-9.21$ ,  $\text{MUR}(\text{ZE})=8400$ ).

The pH and Eh properties of the aqueous solution in the interacting system are always defined in the following way:

$$\text{pH} = -\log_{10} [\text{ACR}(\text{H}+1, \text{AQUEOUS}) * \text{AH}_2\text{O}] \quad \text{Eh} = \text{MUR}(\text{ZE}) / \text{RNF}$$

The symbol AH<sub>2</sub>O is the molecular weight of solvent H<sub>2</sub>O (equals 55.508435) and RNF is the Faraday constant (equals 96485.309).

The activity of the solvent water (ACRH<sub>2</sub>O, A<sub>w</sub>), the osmotic coefficient of aqueous solution (OSMC, O<sub>s</sub>), electronic affinity (A<sub>h</sub>), electronic activity log<sub>10</sub>ACRe (p<sub>e</sub>), ionic strength (IS), total aqueous concentration, in molality (T<sub>M</sub>) and total alkaline concentrations under two definitions (A<sub>t1</sub>/A<sub>t2</sub>) are calculated and listed for each equilibrium state.

POLY3 calculations for mass balances in Thermo-Calc are always based on site-fractions. Consequently, when functions for describing various properties of aqueous solutes are defined, such as molality (ML<sub>i</sub>), activity coefficient (RC<sub>i</sub>) and activity (AI<sub>i</sub>), they should be converted to molality-based quantities:

$$\text{ML}_i = Y(\text{AQUEOUS}, i) * \text{AH}_2\text{O} / \text{YH}_2\text{O}$$

$$\text{RC}_i = \text{ACR}(i, \text{AQUEOUS}) * \text{YH}_2\text{O} / Y(\text{AQUEOUS}, i)$$

$$\text{AI}_i = \text{ACR}(i, \text{AQUEOUS}) * \text{AH}_2\text{O}$$

Here, YH<sub>2</sub>O is the site-fraction of solvent H<sub>2</sub>O and AH<sub>2</sub>O equals 55.508435.

Many more variables, functions and tables can be entered for various purposes. For instance, an equilibrium constant for a homogeneous reaction or a solubility product for a solid dissolution reaction can be entered.

---

## Thermodynamic Data Requirements

In this section:

---

<i>Required Thermodynamic Data</i> .....	10
<i>Including or Excluding the Gas Phase</i> .....	10



## Required Thermodynamic Data

To calculate a Pourbaix diagram, thermodynamic data for at least the following four types of phases must be available:

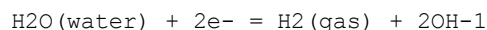
- The aqueous solution phase which applies a certain aqueous solution model. In Thermo-Calc, information about this phase could be retrieved from, for instance, the TCAQ or AQS database (these also include data for the `REF_ELECTRODE` phase that is used for setting the reference state of the standard hydrogen electrode).
- The alloy solution and/or compound phases for the primary matrix phases (and possibly also for the precipitated phases in the alloy. Examples of such phases include FCC\_A1, BCC\_A2, HCP\_A3, SIGMA and CEMENTITE. In Thermo-Calc, information about such phases could be retrieved from, for example, the TCFE database for steels/Fe-alloys, the TCNI database for Ni-based superalloys, the TCAL database for Al-based alloys, the TCMG database for Mg-based alloys, the TCSLD for Sn-/Au-/Bi-/Zn-based solder alloys or the SSOL for general alloys.
- The secondary solid phases that would form as a result of the heterogeneous chemical or electrochemical reactions. These phases could be, for example, oxides, hydroxides, silicates, hydrous silicates, sulphides, sulphates, carbonates, nitrates, phosphates, borates or halides. In Thermo-Calc, information about such phases could be retrieved from, for example, the SSUB database for pure solid compounds or the TCOX database for complex oxide solids.
- The gaseous mixture phase. Information about this phase could be retrieved from, for example, the SSUB database. However, note that it is also possible to perform Pourbaix diagram calculations that ignore the gaseous mixture phase.

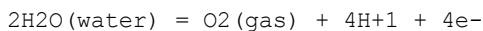
All this thermodynamic data about the various phases must be critically assessed and internally consistent. Furthermore, when the data is retrieved from several databases, the data taken from each database must be consistent with the data taken from the other databases. When Pourbaix diagrams and other diagrams of steel corrosion processes are calculated, it is typically recommended that the TCAQ, TCFE, SSUB and TCOX databases or the AQS, TCFE, SSUB and TCOX are used in combination.

The public PAQ and PAQS databases each contains thermodynamic data for all four phase types and can be used for calculating Pourbaix diagrams. They have been designed specifically for the purpose of demonstrating the POURBAIX module functionality in Thermo-Calc. However, these databases only allow you to perform test calculations for simple cases with major phases in which only a few elements can be considered.

## Including or Excluding the Gas Phase

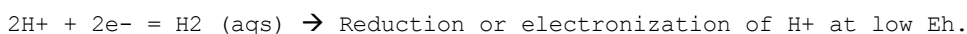
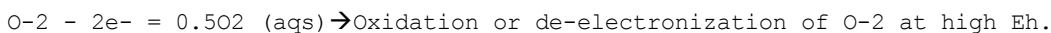
Under defined pressure and temperature conditions, the solvent water's thermodynamic stability limits are determined by the following two electrochemical reactions:



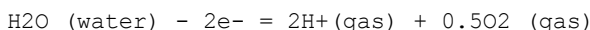
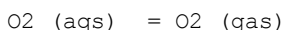


The first reaction describes the formation of H<sub>2</sub>-dominated gaseous mixture, under reducing conditions. The second reaction describes the formation of O<sub>2</sub>-dominated gaseous mixture, under oxidising conditions.

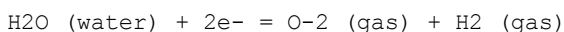
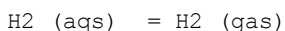
If the system reaches global equilibrium, then the water component is electrolyzed to H<sup>+</sup> and O<sup>2-</sup> at all pH conditions. The degree of electrolysis depends on the pH value in the aqueous solution phase. If Eh gets high enough, then the O<sup>2-</sup> anion is oxidized to O<sub>2</sub> (aq). On the other hand, if Eh gets low enough, then the H<sup>+</sup> cation is reduced to H<sub>2</sub> (aq). The major electrolysis and redox reactions are the following:



At a critically high Eh value under a given pH condition, an aqueous solution phase with a high enough O<sub>2</sub> activity becomes less stable than an O<sub>2</sub>-dominated gaseous mixture phase. At this point, the gas phase replaces the aqueous solution phase in the system. The replacement process can be characterised by the following phase-transformation on the aqueous-gas phase boundary and oxidation of remaining water:



Similarly, at a critically low Eh value under a given pH condition, an aqueous solution phase with a high enough H<sub>2</sub> activity becomes less stable than a H<sub>2</sub>-dominated gaseous mixture phase. At this point, the gas phase replaces the aqueous solution phase in the system, through the following phase-transformation on the aqueous-gas phase boundary and reduction of remaining water:



The phase transformation from an aqueous solution phase to an O<sub>2</sub>- or H<sub>2</sub>-dominated gaseous mixture phase also depends on the total molar Gibbs energies of the phases (which are complex functions of the phase constituents, the temperature and the pressure). The Gibbs energy minimization technique used in Thermo-Calc ensures that the phase transformation is accurately simulated.

The following Pourbaix diagrams show the result of a calculation where the gaseous mixture phase was included. In the upper region (high Eh) and lower region (low Eh), the aqueous solution phase has been oxidized and reduced, respectively, to an O<sub>2</sub>- or H<sub>2</sub>-dominated gaseous mixture phase.

The two example diagrams show that the upper and lower boundaries between the aqueous phase (water) and the gas phase (dominated by either O<sub>2</sub> or H<sub>2</sub>) can shift when solutes dissolve or when the temperature and pressure change.

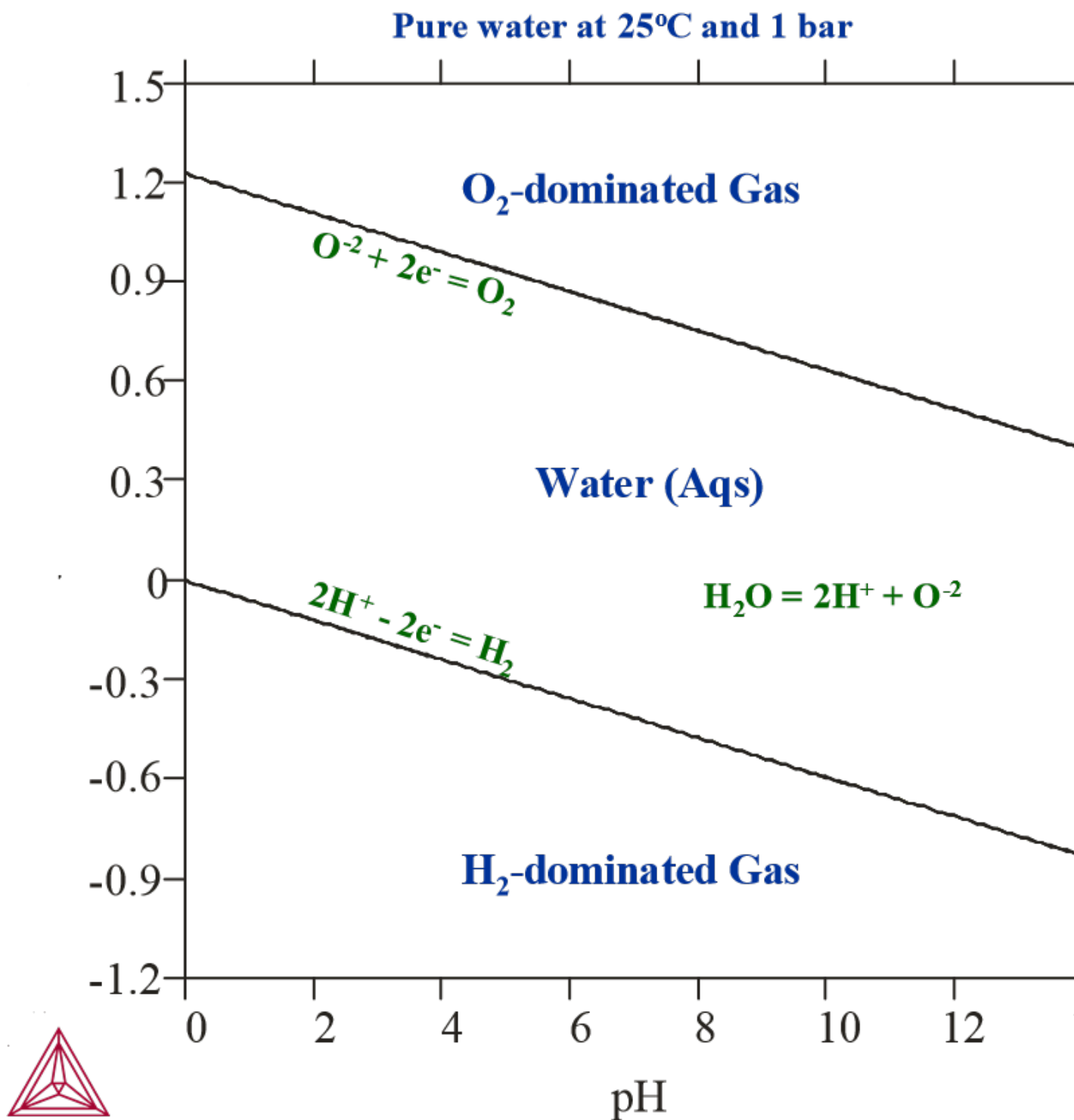
Accordingly, if one does not take a gaseous mixture phase into account when performing a calculation of Pourbaix diagram (as above), then the aqueous solution phase may end up with an extremely high O<sub>2</sub> (aq) concentration at high Eh condition, or an extremely high H<sub>2</sub> (aq) concentration at low Eh

condition. Under either of these two extreme circumstances, the concept of “aqueous solution phase” is no longer valid and consequently no proper aqueous solution model can actually be applied. Therefore, from a restrictive thermodynamic equilibrium point of view, one shall normally include a gaseous mixture phase in an aqueous-bearing heterogeneous interaction system. This is true for all types of equilibrium calculations for an aqueous-bearing heterogeneous interaction system, not only of Pourbaix diagram calculations.

Hence, to perform a completely accurate Pourbaix diagram calculation, the gaseous mixture phase must be taken into account. However, since these electrochemical reactions normally have much higher kinetic barriers and are slower than other electrochemical and chemical reactions in the interaction system, one can sometimes ignore the gaseous mixture phase in the calculation. Note that if the gaseous mixture phase is ignored in this way, then the Pourbaix diagram does not show the H<sub>2</sub>O-stability limiting lines.

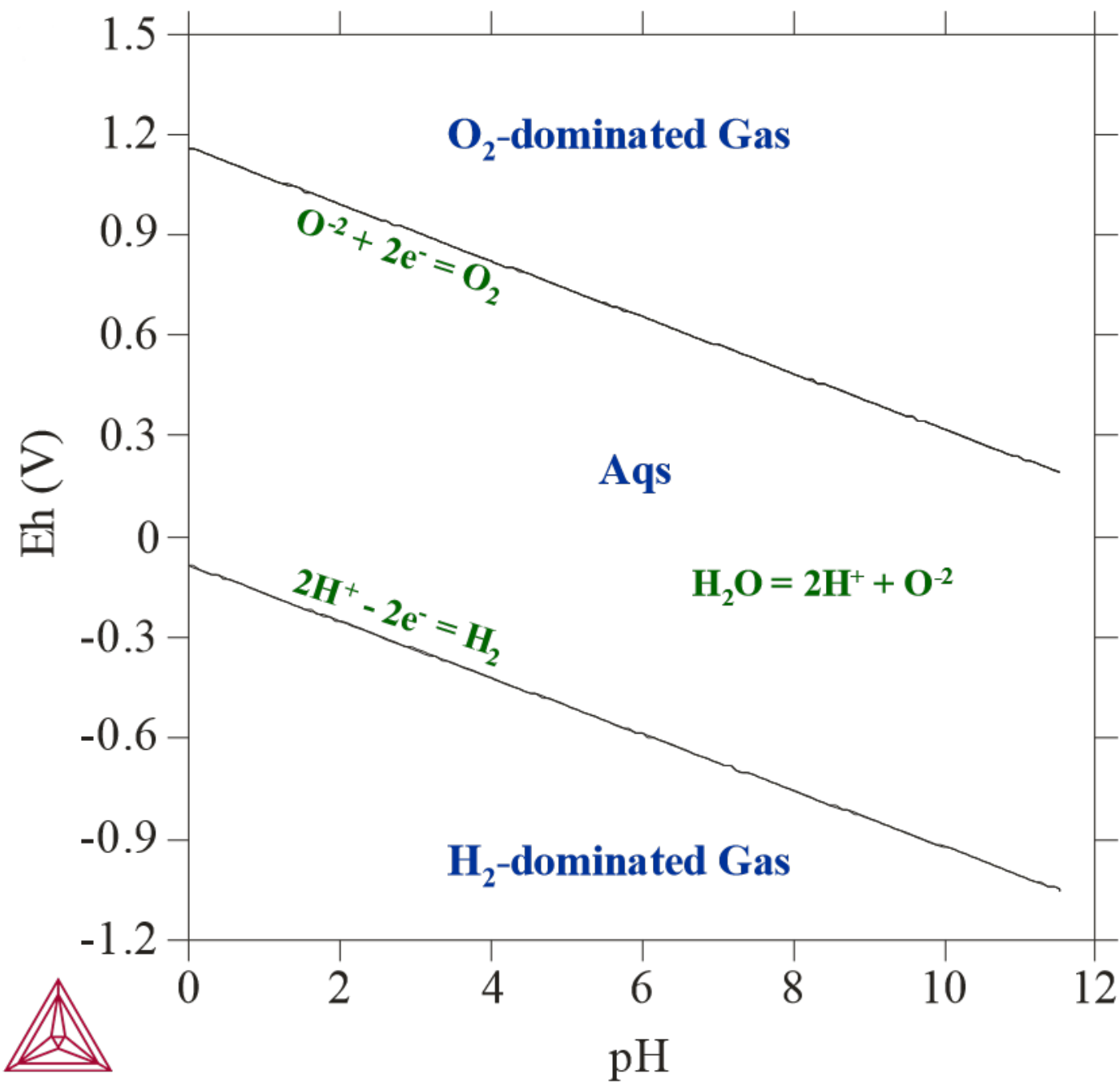
### Example Diagrams

The first diagram is a pH-Eh diagram for pure water at 25°C and 1 bar:



The second diagram is a pH-Eh diagram for 3mNaCl-0.001mCO<sub>2</sub>-0.001mSO<sub>2</sub> aqueous solution at 150°C and 100 bar.

**3mNaCl-0.001mCO<sub>2</sub>-0.001m SO<sub>2</sub> aqueous solution at 150°C and 100**



---

## Examples of Pourbaix Diagrams for Fe

The following two topics are examples of Pourbaix diagrams for Fe. For the first example, the calculations on which the diagrams are based have not taken the gas phase into account. The diagrams in the second example are based on calculations that have taken the gas phase into account.

In this section:

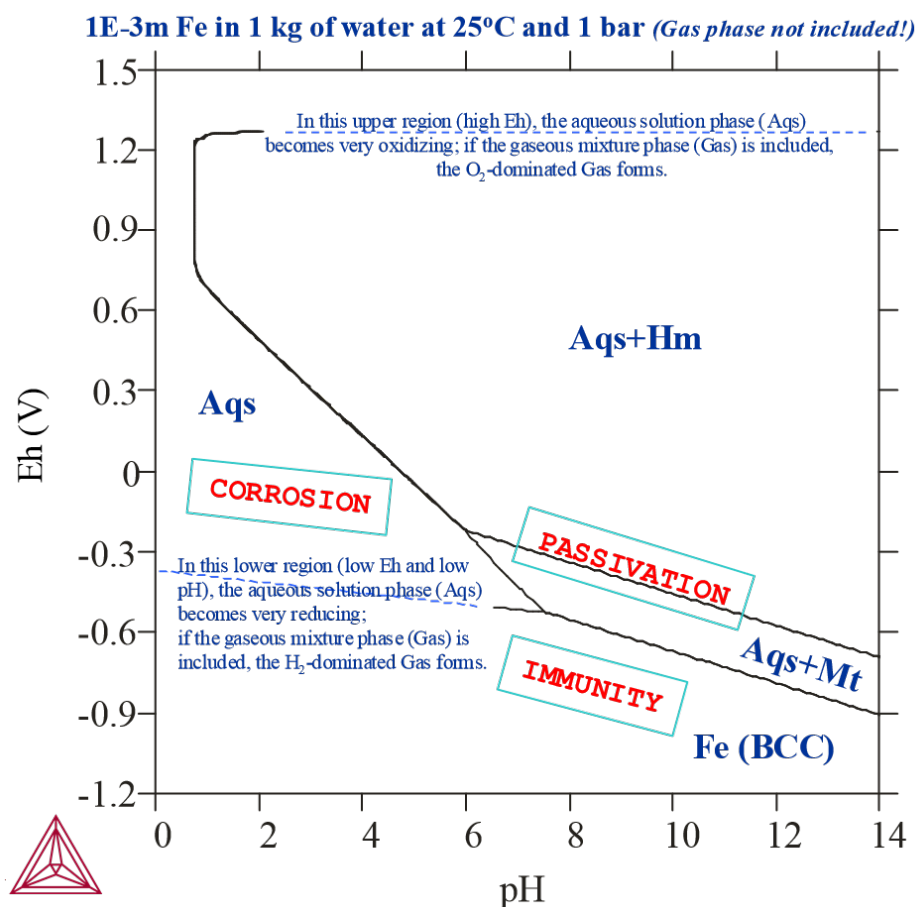
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<i>Pourbaix Diagrams with Gas Phase Excluded</i> .....	<a href="#">16</a>
<i>Pourbaix Diagrams with Gas Phase Included</i> .....	<a href="#">16</a>

## Pourbaix Diagrams with Gas Phase Excluded

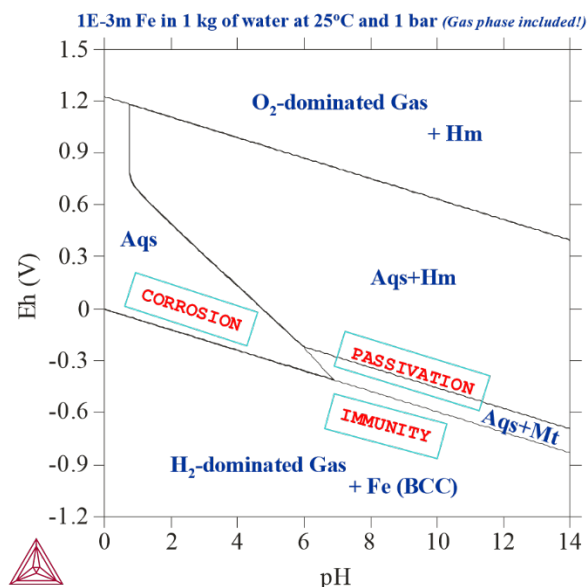
This is an example of a Pourbaix diagram of Fe, in which the gas phase has not been considered in the calculation. The system has 0.001 mole of Fe in 1 kg of pure water at a temperature of 25°C and a pressure of 1 bar. Magnetite (Mt,  $\text{Fe}_3\text{O}_4$ ) and hematite (Hm,  $\text{Fe}_2\text{O}_3$ ) co-exist with the Fe-containing dilute aqueous solution. The formation of magnetite and hematite represent the passivation of iron in the upper right pH-Eh field.

If pH is low and Eh is relatively high, then Fe eventually completely dissolves into the aqueous solution phase. Under conditions of low Eh, Fe remains in its stable solid state, the BCC phase, and neither dissolves into water nor into alternates to Fe (the immunity of Fe).



## Pourbaix Diagrams with Gas Phase Included

With all the possible redox reactions involving the aqueous solution phase and gaseous mixture phase being considered in the equilibrium system, that is, the gaseous mixture phase is included in the calculation, the Pourbaix diagram of Fe in a system with 0.001 mole of Fe in 1 kg of pure water at 25°C and 1 bar.



Comparing this Pourbaix diagram with that from [Basic Settings and Definitions on page 7](#), you can see that both diagrams are for the same interaction system under the same temperature-pressure condition, but the present diagram shows the results of calculations where the gaseous mixture phase has been included. It presents the complete Pourbaix diagram for the defined interaction system, in a full thermodynamic equilibrium. In the upper region (high Eh) and lower region (low Eh), the aqueous solution phase is oxidised and reduced to the O<sub>2</sub>- or H<sub>2</sub>-dominated gas phase. Hematite coexists with the O<sub>2</sub>-dominated gas, while Fe-BCC is stable with the H<sub>2</sub>-dominated gas. The stability field of magnetite may extend slightly into the H<sub>2</sub>-dominated gas region, where it coexists with the gaseous mixture instead of the aqueous solution. Its boundary with Fe (BCC) cannot be drawn due to the absence of aqueous solution phase.

It is not possible to calculate the pH value in both the O<sub>2</sub>- and H<sub>2</sub>-dominated gaseous mixture phase stability regions where the aqueous solution phase is absent. Hence, in a normal Pourbaix diagram, no line is drawn that indicates a phase boundary between the gas phase and the metallic phases or secondary phases (that is, metal-oxides).



---

## Other Examples of Pourbaix Diagrams

In this section:

---

<i>Variations of Pourbaix Diagrams</i> .....	<a href="#">19</a>
<i>Pourbaix Diagrams for Complex Alloys</i> .....	<a href="#">21</a>
<i>Pourbaix Diagram References</i> .....	<a href="#">23</a>

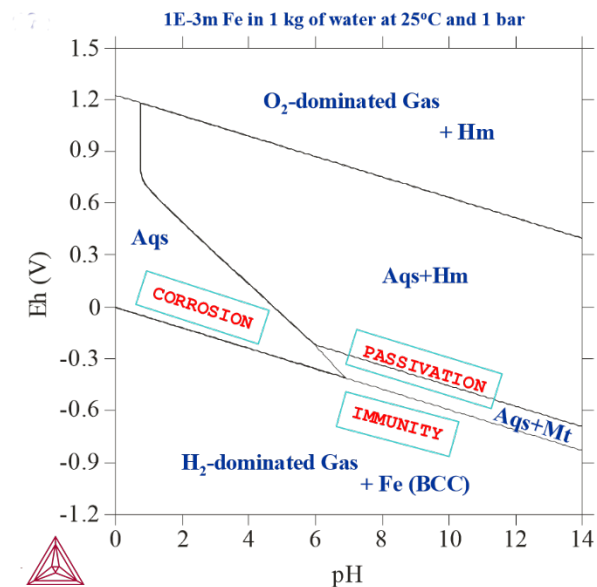
## Variations of Pourbaix Diagrams

The shape of a Pourbaix diagram of an alloy or condensed material and the stability relations of various secondary phases depend upon the following system factors:

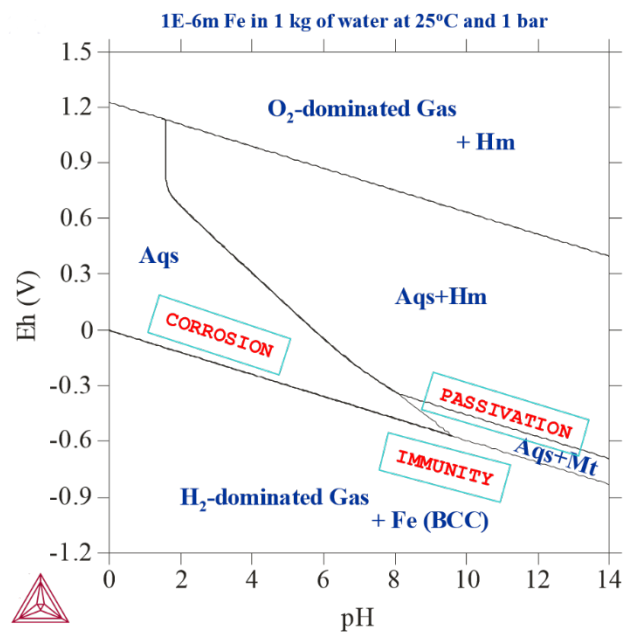
- Initial amount of the alloy or other condensed materials
- Initial composition of the alloy or other condensed materials
- Initial amount of the interacting aqueous solution phase
- Initial composition of the interacting aqueous solution phase
- Temperature and pressure conditions

In the interaction system that the diagrams in *Pourbaix Diagrams with Gas Phase Excluded on page 16* and *Pourbaix Diagrams with Gas Phase Included on page 16* are based on, the initial amount of pure Fe that was taken to have effectively reacted with 1 kg of pure water at 25°C and 1 bar was 0.001 m. The following diagrams are Pourbaix diagrams of Fe where other initial amounts of pure Fe have been used, or where the interacting aqueous solution compositions have been alternated, or the temperature and/or pressure have been changed. Gaseous mixture phases have been included in all the calculations that these diagrams are based on.

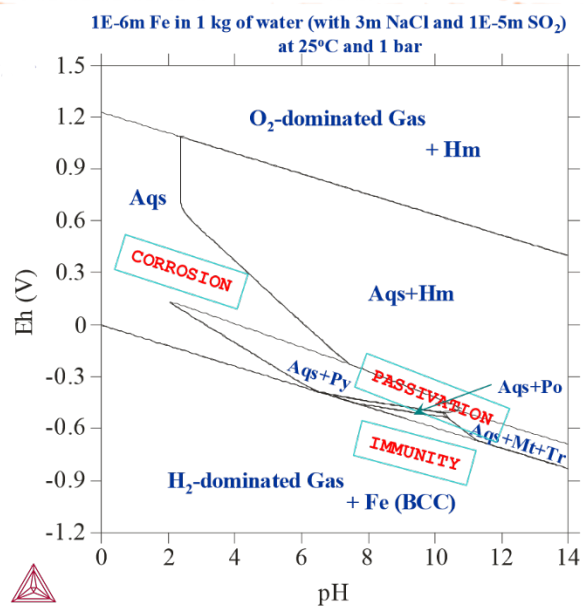
In the first diagram, 1E-3 m Fe actively reacted with 1 kg of pure water at 25°C and 1 bar (as in the calculation in *Pourbaix Diagrams with Gas Phase Included*):



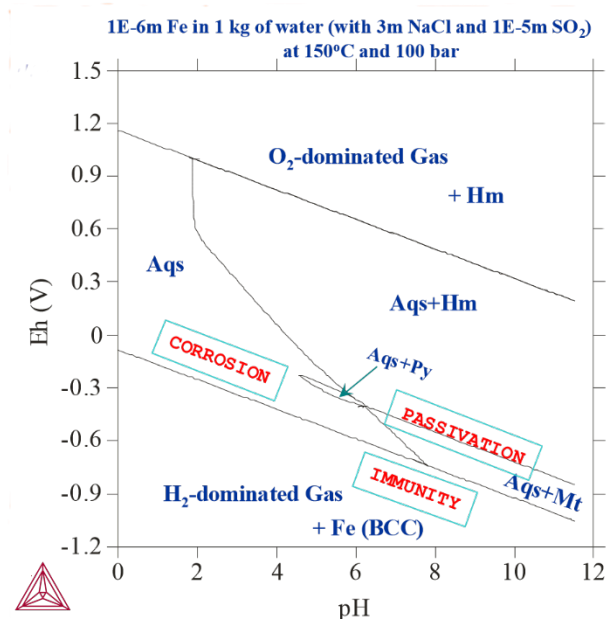
In the second diagram, 1E-6 m Fe actively reacted with 1 kg of pure water at 25°C and 1 bar. Note that the active metal corrosion region gets enlarged as the initial Fe amount decreases from 1E-3m to 1E-6m:



In the third diagram, 1E-6 m Fe actively reacted with 1 kg of water, 3m NaCl and 1E-5 m SO<sub>2</sub> at 25°C and 1 bar. Introducing SO<sub>2</sub> into the system leads to the formation of various metal-sulphides (Py-pyrite, Poppyrrhotite, Tr-troilite). In addition, the passivation region becomes larger.



Finally, in the fourth diagram, 1E-6 m Fe actively reacted with 1 kg of water, 3m NaCl and 1E-5 m SO<sub>2</sub> at 150°C and 100 bar. Here, changing the temperature and pressure affects the stability fields of various Fe-oxides/sulphides.

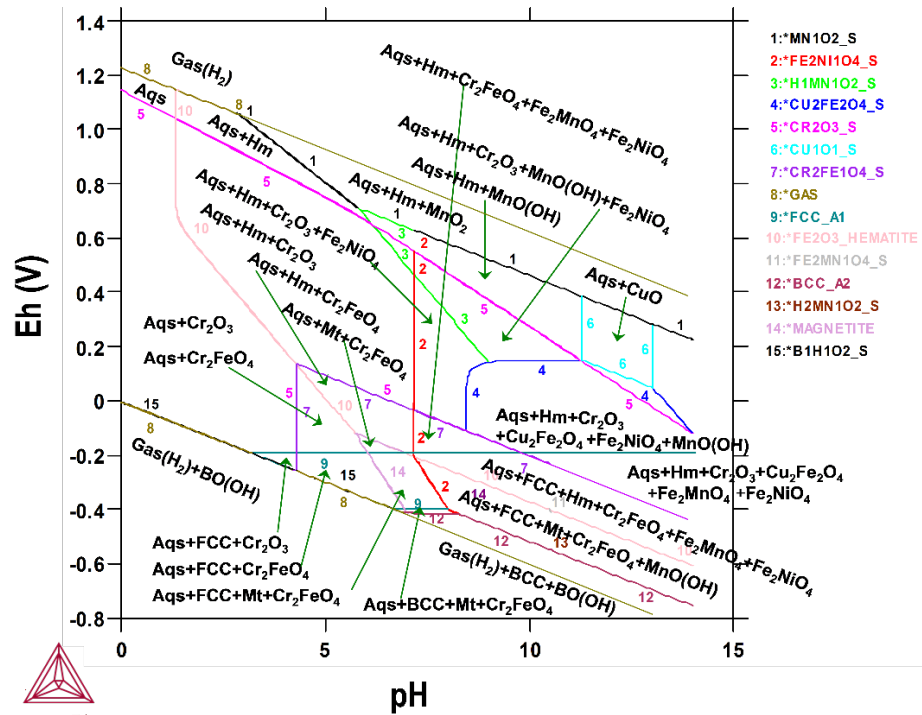


As you can see from the four diagrams, the aqueous-gas phase boundaries shift as the initial bulk compositions, pressure and temperature conditions in the interaction system change.

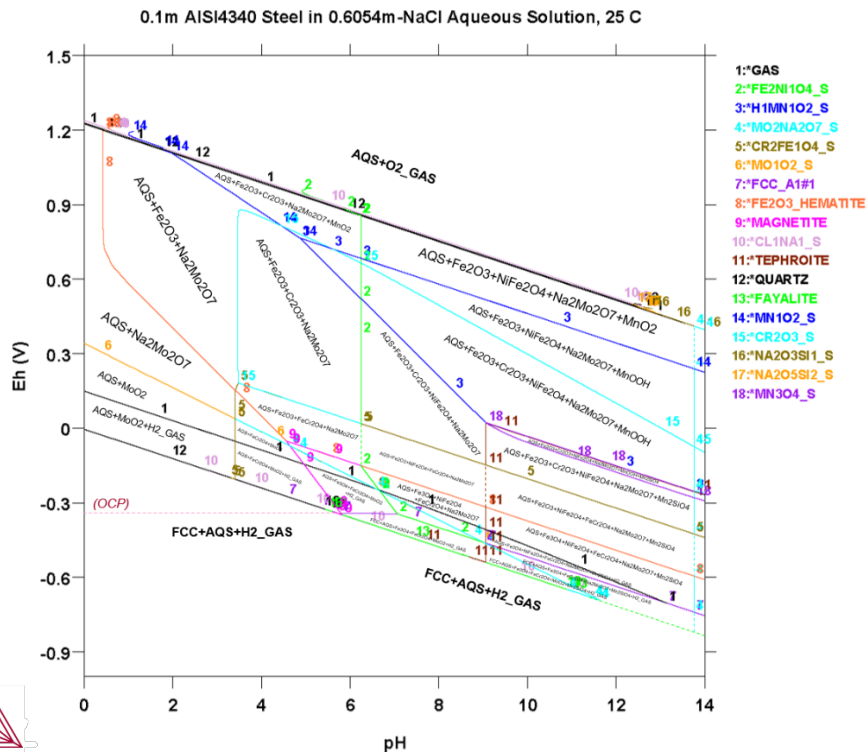
## Pourbaix Diagrams for Complex Alloys

Thermo-Calc can not only be used to simulate how pure metals interact with pure water or simple aqueous solutions under normal pressure and temperature conditions. It can also be used to calculate how complex alloys and concentrated aqueous solutions interact over a very wide pressure, temperature and composition ranges. This is illustrated with the two examples.

The first example is a Pourbaix diagram calculated for the heterogeneous interaction between 0.001 mole of steel (Fe-7.676Cr-5.0Ni-2.1887Mn-1.0Cu [at%]) and 1 kg of water (and with 1.2 m H<sub>3</sub>BO<sub>3</sub>, 0.022 m Li and 0.001 m NH<sub>3</sub>), at 25°C and 1 bar. This application is particularly useful for safety assessments of nuclear reactors and nuclear waste repositories.



The next example is a Pourbaix diagram calculated for the heterogeneous interaction systems between 0.1 mole of AISI4340 stainless steel (Fe-0.80Cr-1.85Ni-0.70Mn-0.25Mo-0.25Si-0.40C [wt%]) and 1 kg of seawater (with the equivalent of 0.6054 m NaCl), at 25°C and 1 bar. This application is particularly useful for failure analysis of petroleum exploitation industry.



---

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# **DATAPLOT User Guide**

**Thermo-Calc Version 2016a**





# Introduction to the DATAPLOT User Guide

In this section:

---

<i>Using this Guide</i> .....	3
<i>About the DATAPLOT Graphical Language</i> .....	3

---

## Using this Guide

The *DATAPLOT User Guide* gives all the details on the graphical language DATAPLOT that a phase diagram or property diagram calculated by Thermo-Calc or a kinetic profile simulated by the Diffusion Module (DICTRA) can be defined.

This guide

- Discusses the important features of the DATAPLOT language.
- Describes the commands to define PROLOGUE and DATASET.
- Several examples and the standard codes for formatting are provided.

A topic introduce the method of formatting DIGLIB symbols in LaTeX documents, for the purpose of necessarily/appropriately referring to the corresponding LaTeX symbols (closest to those DIGLIB symbols which have been plotted on a diagram using the DATAPLOT Graphical Language) in the texts of LaTeX documents for publications/reports.

## About the DATAPLOT Graphical Language

In order to obtain graphical output of any numerical data and informative strings, a graphical language called DATAPLOT was developed in connection with the graphical software DIGLIB. Using this graphical language, you can store information in a normal text file (\*.EXP), which can be plotted as graphical symbols, lines, texts or Greek letters on any plot device support by DIGLIB.

You can generate and plot DATAPLOT (\*.EXP) files together with various calculation and/or experimental results from, for example, phase and property diagrams calculated with the Thermo-Calc software composition profiles or other diagrams simulated by the Diffusion Module (DICTRA).

An EXP file automatically generated by the POST-processor (using the [MAKE\\_EXPERIMENTAL\\_DATAFILE](#) on page 199 command) in the Thermo-Calc software is a DATAPLOT (\*.EXP) file and may contain all types of legal DATAPLOT commands and parameters. With a text editor, you can modify or add some DATAPLOT commands and related parameters in an existing EXP file. This is useful when appending experimental information to calculated/simulated plots, and when specifying user-defined texts, symbols, colors, fonts, filled patterns, diagram types, diagram sizes, symbol/character sizes, titles, special characters, etc.

## DATAPLOT Examples

To help you prepare your EXP (experimental) files to use for your plotted diagrams generated by Thermo-Calc simulations, there are examples of EXP files using the DATAPLOT graphical language standard, which are normally independent of software versions.

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## Using DATAPLOT Graphical Language

In this section:

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<i>DATAPLOT File Structure</i> .....	<i>5</i>
<i>DATAPLOT Language Syntax</i> .....	<i>5</i>
<i>Coordinate Systems</i> .....	<i>5</i>
<i>Graphical Operation Codes</i> .....	<i>6</i>
<i>Tables or Blocks</i> .....	<i>7</i>
<i>Drawing a Polygon</i> .....	<i>8</i>
<i>Drawing an Analytical Function</i> .....	<i>8</i>
<i>Painting of an Enclosed Area</i> .....	<i>8</i>
<i>Writing a Text</i> .....	<i>8</i>
<i>Plotting a Symbol</i> .....	<i>9</i>
<i>Other Commands</i> .....	<i>10</i>
<i>Interactive Plotting</i> .....	<i>11</i>
<i>Formatting DIGLAB Symbols in LaTeX Documents</i> .....	<i>11</i>
<i>LaTeX Formatting Codes</i> .....	<i>12</i>

## DATAPLOT File Structure

A DATAPLOT file is a normal text file with the extension `EXP` that can be created with a text editor or by a program. The file must contain one or more `DATASETS` and possibly also one or more `PROLOGUES`. Each `PROLOGUE/DATASET` is an entity that can be individually selected for plotting.

A `PROLOGUE/DATASET` is identified by a unique positive number in the file. A `PROLOGUE` normally contains various `DATASET` commands for defining information about axis scaling, axis text, axis length, title and so on. A `PROLOGUE` is terminated by another `PROLOGUE` or by the first `DATASET`. This means that all `PROLOGUES` must be placed at the beginning of the file, before the first `DATASET`.

A `DATASET` normally contains `DATASET` commands that are associated to separate data points, as well as with one or more `BLOCKS` of data (calculated or experimental). A `DATASET` is terminated by another `DATASET` command or the end of file.

## DATAPLOT Language Syntax

The DATAPLOT language consists of commands with or without parameters:

```
COMMAND {parameter(s)}
```

The basic graphical command consists of an X/Y coordinate pair and a Graphical Operation Code (`GOC`). With other commands, the interpretation of this basic command can be modified. There are separate commands to draw a polygon or a function and ways to get texts in different fonts.

To edit a DATAPLOT file, the graphical commands can be abbreviated.



A command (with parameters) must not exceed 80 characters. If it is too long (normally as writing necessary codes in a command's parameters for a complex expression), two or more lines can be edited.

## Coordinate Systems

The DATAPLOT language accepts coordinates in three different coordinate systems, which are called *word*, *virtual* and *normalized*.

- The *word* coordinates are selected to represent any kind of data and be of “any” magnitude.
- The *virtual* coordinate system uses centimeters as units. However, the actual size of one unit is dependent on the implementation of the device driver in DIGLIB. It is not recommended to use this coordinate system if different output devices are used for preliminary and final plots.
- The *normalized* coordinate system goes from zero to one. When plotting, you interactively scale each axis by selecting the minimum and maximum word coordinates on the axis. In the normalized coordinate system, the minimum axis value is represented by

zero and the maximum by one. DIGLIB draws a square between the four points (of the X and Y axes) that are determined by the coordinates zero and one in the normalized coordinates.



It is also possible to draw triangular plots as described below. However, in most places, it only references square diagrams. All data points within the minimum and maximum word coordinates are plotted inside this square. DIGLIB also writes tic marks and corresponding word values at such tic marks.

It may be convenient to use normalized coordinates to draw boxes and texts. You can give normalized coordinates outside zero and one if you want to write texts outside the area enclosed by the square. To ensure proper operation outside the normalized box, the clipping must be turned off.

## Graphical Operation Codes

The Graphical Operation Code (GOC) determines how the coordinates are interpreted and what is done at the point determined by the coordinates. For an individual data point, its GOC codes must be given. For each data [BLOCK on page 19](#), you define a default GOC that is used for the whole BLOCK, unless a GOC is explicitly defined for a specific point.

- If *s* is omitted, no symbol is plotted. A number selecting the symbol can optionally follow the character *s*. The DIGLIB software determines which symbol the number represents. See [Plotting a Symbol on page 9](#).
- If any of the other characters are omitted, the default defined for the BLOCK is used. Absolute values imply the current coordinates; relative values mean that these are added to the current coordinates. The GOC must be written without any space between various characters, but the order for the characters is irrelevant.
- If no GOC is defined for a BLOCK, the system default is *MWA*, (Move Word Absolute), i.e., move to the given point that is interpreted as absolute word coordinates. *GOC=DNA* means draw a line from the current point to the new one interpreting the coordinates as normalized. After each draw or move operation, the so-called current point is the new point.
- The [TEXT on page 27](#) following the `'` command is interpreted and expanded by the DIGLIB software, if it includes any `^` operator or [STRING on page 25](#) names using the `~` descriptor. To get PostScript outputs, the TEXT must be edited by the LaTeX Text Formatting Program instead (see [LaTeX Formatting Codes on page 12](#)).

## GOC Character Definitions

The GOC is a combination of the following characters:

Character	Meaning
W, V or N	To use word (W), virtual (V) or normalized (N) coordinates. W is the default.
A or R	XY are absolute (A) or relative (R) values. A is the default.
M or D	To perform a move (M) or draw (D) operation to XY. M is the default.
B	To apply “soft” splines on a line drawn between the coordinate pairs (used only on BLOCK data).
S	To plot default symbol at XY.
S#	To change default symbol to No # symbol and plot it at XY.
`TEXT	To plot TEXT at XY. It must be the last operation in a GOC code. The TEXT following the ' command is interpreted and expanded by the DIGLIB software, if it includes any ^ operator or STRING names using the ~ descriptor.

## Tables or Blocks

In many cases, you have (calculated or experimental) data in the form of tables, and want to plot one or several columns as X-axis and one or more columns as Y-axis. A single table can contain many sets of data records of the same kind of information for a specific data [BLOCK on page 19](#). There can be many data BLOCKS in a [DATASET on page 19](#).

By enclosing these tables in a data BLOCK, you can select which column(s) is the X-axis and which is the Y-axis. For example,

```
BLOCK X=C1; Y1=C3; Y2=C2; GOC=C4,DAW
```

Where the X-axis values are in column 1, the Y-axis values are in columns 2 and 3, and any GOC codes are in column 4. The default GOC for this BLOCK is Draw Absolute Word. The GOC code inside the table is only necessary if the default GOC is not applicable.

A more elaborate use of the table is shown in this example:

```
BLOCK X=C3; Y=1E3/(C3+273); GOC=C8,MAWS1
```

Where the X-axis values are in column 3, the Y-axis values are in column 1 with some additional calculations applied. Any GOC is in column 8, and the default GOC is Move Absolute Word and plot the symbol no. 1.

Columns in a table must be separated by one or more space characters and do not have to be justified.

It is possible to have tables with mixed text and numbers, but each word followed by a space is counted as one column. The columns used for plotting also must be numerical. An example of a legal line in a table is

```
298.15 This_is_the_second_column 11.5 This_is_the_fourth_column
```



A line in the table must not exceed 80 characters. A BLOCK must be terminated by a line with the [BLOCKEND on page 20](#) command.

## Drawing a Polygon

Normally, each point is written on a separate line. But in order to draw a line in a more compact way, use the command [DRAWLINE on page 21](#). DRAWLINE is followed by a couple of X/Y number pairs. The X/Y pairs must be separated by a space, and there must be a comma sign between the X and Y values. DRAWLINE makes a move operation to the first pair of X/Y coordinates, and then draws a line among all pairs up to the last one. All pairs must fit on one line of 80 characters, but there can be several consequent DRAWLINE commands.

## Drawing an Analytical Function

Use a [BLOCK on page 19](#) command to set an axis to a function. It is not necessary to use a value from any column in order to compute the function value to be plotted. Use the [FUNCTION on page 27](#) command to plot a function with an even increment of the independent variable.

## Painting of an Enclosed Area

Use the [PAINT on page 27](#) command to paint or fill an area in a specified pattern in the plot. Available patterns are determined by the DIGLIB software. A related command to PAINT is [PCFUNCTION on page 27](#).

## Writing a Text

Use the [TEXT on page 27](#) command to write a text at the current point. You can write a text at any X/Y pair by appending a single quote followed by the text on the same line. For example:

```
1.1 1.0 NAM'This is a text
```

writes `This is a text` at the normalized coordinates (1.1, 1.0).

Use the command [FONT on page 24](#) to select the font used for the text, and [CHARSIZE on page 22](#) to select the size of the characters. Set this size of the symbols with [SYMBOLSIZE on page 22](#).

If a text or a single character should be of a different font than all the other text, or to use subscripts or superscripts in a text, use the ^ operators or STRING command to create the text. The command [STRING on page 25](#) stores the text in a specified variable that includes all text-formatting information defined by the DIGLIB software. See [Example 3 – Using Strings and Various Line Types on page 32](#) and [Example 5 – Use Included Files for Predefined Symbols on page 34](#).

However, if a graphical output is done on a PostScript device using the PostScript hardcopy fonts, special text formatting codes as [LaTeX Formatting Codes on page 12](#) should be used and the STRING formatting syntax is then not valid.

## Plotting a Symbol

As described in [Graphical Operation Codes on page 6](#), a GOC code in a data BLOCK may contain an `S` option to plot a symbol for an X/Y pair or the same symbols for the data BLOCK. A number selecting the symbol can optionally follow the character `S`. You can plot a symbol at any current X/Y position by appending a quote specified by the symbol number in the GOC code (e.g., `1.1 1.0 MANS5' This is a text`).

You can also insert DIGLIB symbols into LaTeX-edited documents.

### DIGLIB symbols available in Thermo-Calc

The image summarizes all the standard symbols available in the DIGLIB software. A default symbol is the current symbol in the run of the software (it is usually the No 1 symbol if the POST-processor is switched on for the first time). `S` (i.e., `#` is not specified) means that the current symbol is plotted. `S0` (i.e., `#=0`) means that no symbol is plotted.

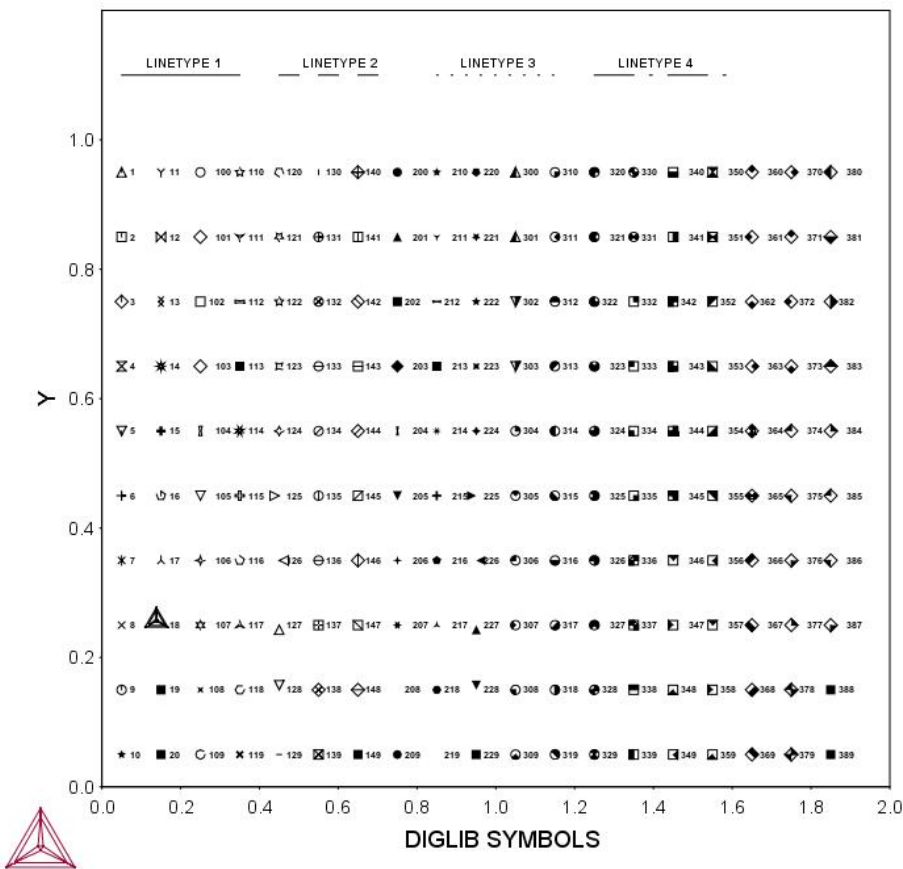


All the DIGLIB symbols work properly and give good output results for the PostScript format.



## DIGLIB Symbols

2015.10.30.10.35.27  
UNKNOWN:



## Other Commands

Use the [LINETYPE on page 21](#) command to define line types as solid, long dashed, short dashed or dotted. If you are using a color device, use the [COLOR on page 22](#) command to change color of the lines. On some black and white devices, colors are simulated with different width and dashing of the lines.

- Use the [CLIP on page 20](#) command to change the default where all data outside the normalized coordinates zero and one are not plotted.
- When plotting symbols representing various experimental data, it is important that the symbols are centered around the coordinate values.
- Use the [ATTRIBUTE on page 20](#) command to change the coordinates where text is displayed. The default is the lower left corner of the first character in the text.
- Use the [INCLUDE on page 28](#) command to create libraries with texts and include these in similar plots.

- The dollar sign \$ as the first character of a line stands for a comment character, which means the whole line is ignored when plotting.

## Interactive Plotting

The DATAPLOT file is read into the POST module in the workspace with [APPEND\\_EXPERIMENTAL\\_DATA](#) on page 192 or [QUICK\\_EXPERIMENTAL\\_PLOT](#) on page 201. These commands ask for the name of the DATAPLOT file and also which PROLOGUE(S) and DATASET(S) are to be plotted.

See the *Thermo-Calc Command Mode Reference Guide* for details about these commands.

By giving the PROLOGUE/DATASET number as -1, you get a list of the available PROLOGUES/DATASETS in the file. Note that if DATASET 0 is in a DATAPLOT file, its data is always used even if other DATASETS are chosen.

## Formatting DIGLIB Symbols in LaTeX Documents

When using the LaTeX editor, you can use the DIGLIB symbols in texts and in figures. This then refers to the corresponding LaTeX symbols (closest to those DIGLIB symbols which are plotted on a plot using the DATAPLOT Graphical Language) in the texts of LaTeX documents for publications/reports.

This topic shows how to generate some DIGLIB symbols in texts, through the attached LaTeX source file and its converted jpg file.

### DIGLIB\_Sym.tex

```
\documentclass[dvips,12pt]{article}

\textwidth 165mm

\textheight 225mm

\oddsidemargin 1mm

\evensidemargin 1mm

\topmargin 1mm

%%\usepackage{amssymb}

%% next replace amssymb and to get uetimes

\usepackage{utopia}{mathdesign}

\usepackage{rotating}

\usepackage[latin1]{inputenc}

\usepackage{graphics}

\usepackage{graphicx,subfigure}% with figures

%\usepackage[draft]{graphicx}% without figures

\usepackage{subfigure}% with figures

\topmargin 1mm

\oddsidemargin 1mm
```

---

```

\evensidemargin 1mm

\begin{document}

{\Large \bf Diglib symbols and their corresponding LaTeX symbols}

\vspace{5mm}

```

The information below gives the closest corresponding LaTeX symbol. All symbols (except +) must be generated in math mode. Most of these require the package `amssymb`, i.e., you need a directive `usepackage{amssymb}` in the preamble. Two of the symbols require the more extensive `mathdesign` that can be included with `usepackage[utopia]{mathdesign}`.

```

\vspace{5mm}

{\Large

\begin{tabular}{llll}
Diglib & Latex & Latex name & Note\\
1&  $\vartriangle$  & \backslash$vartriangle & amssymb \\
2&  $\square$  & \backslash$\square & \\
3&  $\huge \diamond$  & \backslash$diamond & size \backslash$Large \\
4&  $\udtimes$  & \backslash$udtimes & mathdesign \\
5&  $\triangledown$  & \backslash$\triangledown & amssymb \\
6& + & normal + & \\
7&  $\ast$  & \backslash$\ast & amssymb \\
8&  $\times$  & \backslash$\times & \\
9&  $\huge \circ$  & \backslash$\circ & size \backslash$Large \\
10&  $\huge \star$  & \backslash$\star & size \backslash$Large, amssymb \\
11&  $\curlyvee$  & \backslash$\curlyvee & amssymb \\
12&  $\Join$  & \backslash$\Join & \\
13& - & nothing similar, overlapping & > < \\
14& - & nothing similar, 10-edged star & \\
15&  $\maltese$  & \backslash$\maltese & mathdesign \\
16& - & nothing similar, a pentagon & \\
17&  $\curlywedge$  & \backslash$\curlywedge & amssymb \\
\end{tabular}}

\end{document}

```

## LaTeX Formatting Codes



For a list of supported LaTeX commands, see:

<http://www2.ph.ed.ac.uk/snuggletex/documentation/math-mode.html>



By default when using the LaTeX command, you are in math mode and Thermo-Calc automatically interprets the entered text as math. The above link uses the dollar sign (\$) in all the examples but this is NOT required. For example, if you enter  $E=mc^2$  this is displayed including the \$ instead of the equation.



As of Thermo-Calc 2015a the LTEXT text formatting is replaced by LaTeX. For existing users who may have plots and files that use the LTEXT format, and especially when using Console Mode, the following examples show the command changes from LTEXT and its LaTeX equivalent:

### LTEXT vs LaTeX Commands for Labels

Symbol or text format	LTEXT	LaTeX
Subscripts in an axis text	S-A-TEXT Y N Mole-fraction Al <sup>DO2</sup> O <sup>DO3</sup>	S-A-TEXT Y N \latex Mole-fraction Al_ 2O_3
Label with subscript	add .13 .15 n c-ZrO <sup>DO2</sup>	add .13 .15 n \latex c-ZrO_2
Greek symbol	ADD .05 .50 N ^GRd	ADD .05 .50 N \latex \delta

---

## PROLOGUE Commands

In this section:

---

<i>PROLOGUE</i> .....	<i>15</i>
<i>XSCALE</i> .....	<i>15</i>
<i>YSCALE</i> .....	<i>15</i>
<i>XTEXT</i> .....	<i>15</i>
<i>YTEXT</i> .....	<i>15</i>
<i>XTYPE</i> .....	<i>15</i>
<i>YTYPE</i> .....	<i>16</i>
<i>XLENGTH</i> .....	<i>16</i>
<i>YLENGTH</i> .....	<i>16</i>
<i>TIC_TYPE</i> .....	<i>16</i>
<i>TITLE</i> .....	<i>16</i>
<i>DIAGRAM_TYPE</i> .....	<i>17</i>

## PROLOGUE

PROLOGUE is the beginning of a number of consequent lines of user-defined diagram layout commands. The lines are displayed with the `optional text` when using the `-1` option in the POST-processor as prompted for the PROLOGUE number with [APPEND\\_EXPERIMENTAL\\_DATA](#) on page 192 or [QUICK\\_EXPERIMENTAL\\_PLOT](#) on page 201.

Syntax	PROLOGUE # optional text
	# is an unsigned integer identifying the PROLOGUE.

## XSCALE

XSCALE sets the scaling in word coordinates of the X-axis.

Syntax	XSCALE min max
	min and max are real numbers.

## YSCALE

YSCALE sets the scaling in word coordinates of the Y-axis.

Syntax	YSCALE min max
	min and max are real numbers.

## XTEXT

XTEXT sets the X-axis text.

Syntax	XTEXT text
	text is an arbitrary text string that may contain text-formatting codes.

## YTEXT

YTEXT sets the Y-axis text.

Syntax	Y TEXT text
	text is an arbitrary text string that may contain text-formatting codes.

## XTYPE

XTYPE sets the X-axis type as linear (default), logarithmic or inverse.

Syntax	XTYPE type
	type is a character string reading LIN, LOG or INV.

## YTYPE

YTYPE sets the Y-axis type as linear (default), logarithmic or inverse.

Syntax	Y TYPE type
	type is a character string reading LIN, LOG or INV.

## XLENGTH

XLENGTH sets the X-axis length to approximately # centimeters.

Syntax	XLENGTH #
	# is a positive real number (the approximate X-axis length in centimeters).

## YLENGTH

YLENGTH sets the Y-axis length to approximately # centimeters.

Syntax	Y LENGTH #
	# is a positive real number (the approximate Y-axis length in centimeters).

## TIC\_TYPE

TIC\_TYPE sets the relative length of the tic marks.

Syntax	TIC_TYPE #
	# is a real number. Default value is 1. Negative number gives tics on the inside of the diagram frame. 0 gives no tics.

## TITLE

TITLE sets the title text string to be printed above the diagram.

Syntax	TITLE text
	text is an arbitrary text string that may contain text-formatting codes

## DIAGRAM\_TYPE

DIAGRAM\_TYPE sets the diagram type to square (the default) or triangular.

Syntax	DIAGRAM_TYPE type plot_3rd_axis clip_along_third-axis
	type is a character string reading SQUARE (default) or TRIANGULAR. If type reads TRIANGULAR, then two additional parameters are given: plot_3rd_axis and clip_along_third-axis that are character strings reading YES or NO.



---

## DATASET Commands

In this section:

---

<i>DATASET</i> .....	19
<i>BLOCK</i> .....	19
<i>BLOCKEND</i> .....	20
<i>DATAPoint</i> .....	20
<i>CLIP</i> .....	20
<i>ATTRIBUTE</i> .....	20
<i>LINETYPE</i> .....	21
<i>DRAWLINE</i> .....	21
<i>CHARSIZE</i> .....	22
<i>SYMBOLSIZE</i> .....	22
<i>GLOBALSIZE</i> .....	22
<i>COLOR</i> .....	22
<i>FONT</i> .....	24
<i>STRING</i> .....	25
<i>TEXT</i> .....	27
<i>FUNCTION</i> .....	27
<i>PCFUNCTION</i> .....	27
<i>PAINT</i> .....	27
<i>INCLUDE</i> .....	28

---

## DATASET

DATASET indicates the beginning of a number of consequent lines comprising a set of user-defined data. The DATASET lines are displayed on the terminal along with the `optional text` when using the `-1` option in the POST-processor as prompted for the DATASET number in the [APPEND\\_EXPERIMENTAL\\_DATA](#) on page 192 or [QUICK\\_EXPERIMENTAL\\_PLOT](#) on page 201 command.

Syntax	DATASET # optional text
	# is an unsigned integer identifying this set of data.

## BLOCK

BLOCK defines how the following numeric data block shall be interpreted. The definitions of X and Y coordinates may also be expressed as a function of the column values, making it possible to perform transformations.

Syntax	BLOCK X&=C#; ...; Y&=C#; ...; GOC=C#,@@@...
	&' are optional unsigned integers that make it possible to plot several (maximum 9) X- or Y- axis columns. #' are unsigned integers identifying the column numbers. The column number # in "GOC=C#" is the location of any possible GOC codes in the current data BLOCK; @@@ stands for the default Graphical Operation Code (GOC) for the current BLOCK. The GOC code inside the current table is only necessary if the current default GOC is not applicable.

## GOC Characters

The GOC is a combination of the following characters:

Character	Meaning
W, V or N	To use word (W), virtual (V) or normalized (N) coordinates. W is the default.
A or R	XY are absolute (A) or relative (R) values. A is the default.
M or D	To perform a move (M) or draw (D) operation to XY. M is the default.
B	To apply "soft" splines on a line drawn between the coordinate pairs (used only on BLOCK data).
S	To plot default symbol at XY.
S#	To change default symbol to No # symbol and plot it at XY.

Character	Meaning
'TEXT	To plot TEXT at XY. It must be the last operation in a GOC code. The TEXT following the ' command is interpreted and expanded by the DIGLIB software, if it includes any ^ operator or STRING names using the ~ descriptor.

## BLOCKEND

Syntax	BLOCKEND
	BLOCKEND terminates the local definition of the graphical operation code defined by the earlier BLOCK command.

## DATAPPOINT

DATAPPOINT is not a DATASET command, but the basic DATAPLOT command (see synopsis below) performs an action at the current point determined by the specified X/Y- coordinates. A DATASET may contain various data points, in addition to one or more data [BLOCK on the previous pages](#). Such data points are separated and independent on each other.

Syntax	X Y GOC
	X and Y are unsigned real numbers identifying the X/Y-coordinates for the current data point. GOC stands for Graphical Operation Code (GOC) for the current point. Legal GOC characters.
	<p><b>Example</b></p> <pre>0.7 0.95 N'Example 6 0.5 0.08 MNA'E^FS18^SQ(^SK^FS10A+5#8*C#^FS10 -!a^FS18)^FS11+B^DIa#b#S</pre>

## CLIP

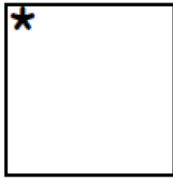
CLIP turns clipping on or off. If it is OFF, it allows output outside the ordinary plot area defined by normalized coordinates zero and one.

Syntax	CLIP CLP
	clp is a character string reading ON or OFF.

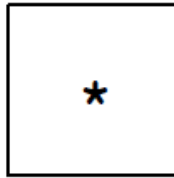
## ATTRIBUTE

ATTRIBUTE specifies where the current XY position is in the character or symbol plotbox.

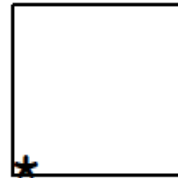
Syntax	ATTRIBUTE
Prompts	attribute
	attribute may be TOP, CENTER or BOTTOM. ATTRIBUTE CENTER is default for symbols; ATTRIBUTE BOTTOM is default for characters.



TOP



CENTER



BOTTOM

## LINETYPE

LINETYPE redefines the current linetype in the plot.

Syntax	LINETYPE #
	<p># must be an unsigned integer. Legal linetypes are (for both normal graphical outputs and for PostScript formats):</p> <ul style="list-style-type: none"> <li>• Solid (default)</li> <li>• Long dashed</li> <li>• Short dashed</li> <li>• Dotted</li> </ul>

## DRAWLINE

DRAWLINE draws a line starting at (x1,y1) to (xn,yn) through (x2,y2)  $\rightarrow$  (x(n-1), y(n-1)).

Syntax	DRAWLINE x1,y1 x2,y2 .... xn,yn												
	<p>x and y may be reals or integers of any value. This is the same as connecting all points in a table:</p> <table><tr><td>x1</td><td>y1</td><td>M</td></tr><tr><td>x2</td><td>y2</td><td>D</td></tr><tr><td>...</td><td>...</td><td>D</td></tr><tr><td>xn</td><td>yn</td><td>D</td></tr></table>	x1	y1	M	x2	y2	D	...	...	D	xn	yn	D
x1	y1	M											
x2	y2	D											
...	...	D											
xn	yn	D											

## CHARSIZE

CHARSIZE redefines the default size of the characters in the plot. The character size has an initial default value, which may vary with the current font setting and the output device (the plot format).

Syntax	CHARSIZE \$\$
	\$\$ must be an unsigned real.

## SYMBOLSIZE

SYMBOLSIZE redefines the current symbol size setting. The symbol size has an initial default value.

Syntax	SYMBOLSIZE \$\$
	\$\$ must be an unsigned real.

## GLOBALSIZE

GLOBALSIZE redefines the default global size of the plot. The global size has an initial default value.

Syntax	GLOBALSIZE \$\$
	\$\$ must be an unsigned real.

## COLOR

COLOR redefines the current color setting. There are 22 legal color codes (from 0 to 21).

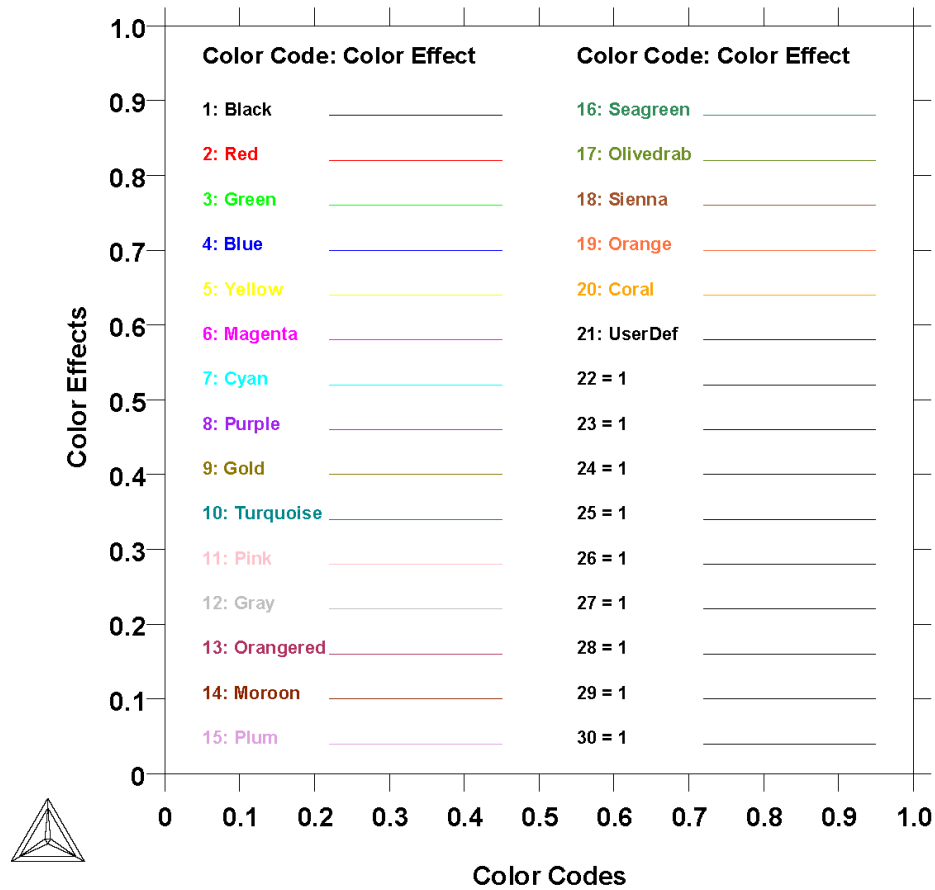
Syntax	COLOR code
	code is an unsigned integer number (from 0 to 21) identifying the color, or a character string specifying the color.

### DIGLIB Color Codes

Code	Color	Equivalent Character
0	Background	Invisible
1	Black	Normal
2	Red	Very_Thick
3	Green	Thin
4	Blue	Thick

Code	Color	Equivalent Character
5	Yellow	Very_Thin
6	Magenta	Dashed
7	Cyan	Dotted
8	Purple	
9	Gold	
10	Turquoise	
11	Pink	
12	Gray	
13	Orangered	
14	Maroon	
15	Plum	
16	Seagreen	
17	Olivedrab	
18	Sienna	
19	Orange	
20	Coral	
21	UserDef	
22 and higher	Any digit larger than 21 has the color effect as 1 (black).	

### DIGLIB Color Effects



## FONT

FONT redefines the default font setting in the POST-processor.

Syntax	FONT #
	# is an unsigned integer.

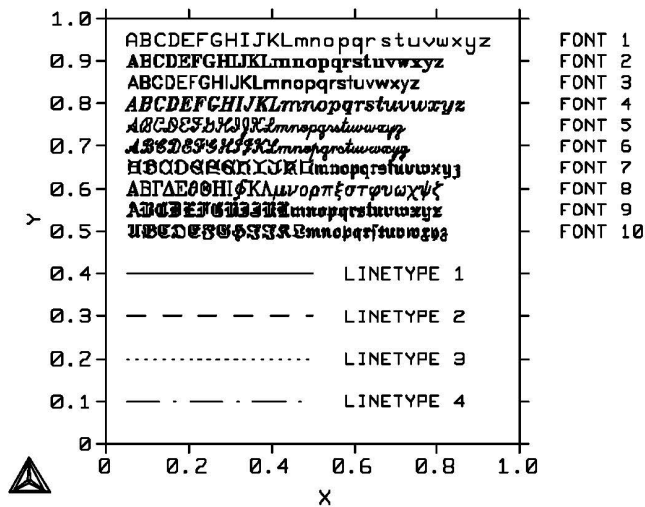
### Font Numbers

Number	Font Name
1	Cartographic Roman (the default)
2	Bold Roman script
3	Bold Roman
4	Bold italic
5	Script

Number	Font Name
6	Bold script
7	UNCIAL
8	Bold Greek
9	Gothic English
10	Gothic Greek

### Examples of all the DIGLIB fonts and line types

THERMO-CALC (2001.08.21:10.53) : DIGLIB Fonts



## STRING

STRING defines a string containing a text and operation codes (e.g., to change the default font settings).



<b>Syntax</b>	<pre>STRING name text_with_each_character_in_ ^S#^G^F#^U#^D#^R#^L#^N</pre>
	<p>name is a valid alphanumeric name (variable) to represent the text including all text formatting codes. It is highly recommended that all the characters in the name are in CAPITAL CASE (e.g. ACA2SO4); otherwise, the defined STRING can be incorrectly plotted.</p> <p>text_with_each_character_in_ ^S#^G^F#^U#^D#^R#^L#^N</p> <p>means the text is coded with each of its characters (and/or numeric numbers) that are formatted with various operators (^S#, ^G, ^F#, ^U#, ^D#, ^R#, ^L# and/or ^N). #' are unsigned integers. ^ is the caret character and does not mean a control character. Between an # (in an operator) and a numeric number (as a part of the text), there must always be a comma sign ( , ) or the number is not plotted in the text, because the # with the number is interpreted as another incorrect #. In some of the commands, #=0 resets the option to previous (or default) value.</p>

### String operation codes in the DIGLIB software

For the PostScript hardcopy fonts, these operation codes are not valid; see [LaTeX Formatting Codes](#) on page 12:

Operator	Operation
^S#	Set character size to size #
^G	Set font to Greek
^F#	Set font to font number #
^U#	Move up # units
^D#	Move down # units
^R#	Move right # units
^L#	Move left # units
^N	Do not move, remain at current

### Examples

```
STRING Alpha1 ^Ga^F0^D0^S8,1^S0^U0
```

is set to  $\alpha_1$

```
STRING M23C6 M^D0^S8,23^S0^U0C^D0^S8,6^S0^U0
```

is set to  $M_{23}C_6$

```
STRING ACA2CO3 ^Ga^F0^D0^S8Ca^D0^S4,2^S0^U0^S8CO^D0^S4,3^S0^U0
```

is set to  $\text{Ca}_2\text{CO}_3$

## TEXT

TEXT outputs, at the current position, the text following the keyword TEXT or the text in the string `string_name` that is defined with [STRING](#) on page 25.

Syntax	TEXT text or ~string_name
	It is possible to mix ^ operators and previously defined string names using the ~ operator.

## FUNCTION

FUNCTION defines and plots a user-defined function.

Syntax	FUNCTION Y=f(X); start end number_of_XY_pairs; GOC; FUNCTION X=f(Y); start end number_of_XY_pairs; GOC;
	f(X) or f(Y) are legal mathematical functions of X or Y, understandable by a FORTRAN program. start and end are unsigned real numbers, and number_of_XY_pairs an unsigned integer. GOC is a legal graphical operation code as defined with <a href="#">BLOCK</a> on page 19.

## PCFUNCTION

PCFUNCTION appends a user-defined function to the current path. It is used with [PAINT](#) below.

Syntax	PCFUNCTION Y=f(X); start end number_of_XY_pairs; GOC; PCFUNCTION X=f(Y); start end number_of_XY_pairs; GOC;
	f(X) or f(Y) are legal mathematical functions of X or Y, understandable by a FORTRAN program. start and end are unsigned real numbers, and number_of_XY_pairs an unsigned integer. GOC is a legal graphical operation code as defined with <a href="#">BLOCK</a> on page 19.

## PAINT

PAINT paints the area enclosed by the current path in the current pattern. The current path starts at the last MOVETO given and includes all subsequent DRAWs. This command only works for the PostScript format (as graphical files or on printed hardcopy).



Also see [PCFUNCTION](#) above.

Syntax	PAINT <code> <video> <mode>
	<p>&lt;&gt; denotes optional parameters. To set a new current pattern, supply any or all of the optional parameters.</p> <ul style="list-style-type: none"><li>• &lt;code&gt; is a single letter 0-9, A-Z or a-t (if &lt;code&gt;=t, also supply a space and a number in the range 0.00-1.00). The default is 0.</li><li>• &lt;video&gt; is a string reading NORMAL (the default) or INVERSE.</li><li>• &lt;mode&gt; is a string reading TRANSPARENT (the default) or OPAQUE.</li></ul>

## INCLUDE

INCLUDE adds a file into the current input stream See [Example 5 – Use Included Files for Predefined Symbols](#) on page 34.

Syntax	INCLUDE filename
	filename is a legal filename (with its correct path) for the operation system.

---

## Examples of DATAPLOT Files and Outputs

In this section:

---

<i>Example 1 – Draw Lines and Symbols .....</i>	<i>30</i>
<i>Example 2 – Draw Polygons and Symbols .....</i>	<i>31</i>
<i>Example 3 – Using Strings and Various Line Types .....</i>	<i>32</i>
<i>Example 4 – Draw Curves Defined by Functions .....</i>	<i>33</i>
<i>Example 5 – Use Included Files for Predefined Symbols .....</i>	<i>34</i>
<i>Example 6 – Plot Triangular Diagrams for Ternary Systems .....</i>	<i>37</i>
<i>Example 7 – Color Codes and Effects .....</i>	<i>41</i>

## Example 1 – Draw Lines and Symbols

```

$DATAPLOT Example 1

PROLOG 1 EXAMPLE 10<X<100, 0<Y<100

XSCALE0.00000100

YSCALE0.00000100

XTYPE LINEAR YTYPE LINEAR

XLENGTH11.5000

YLENGTH11.5000

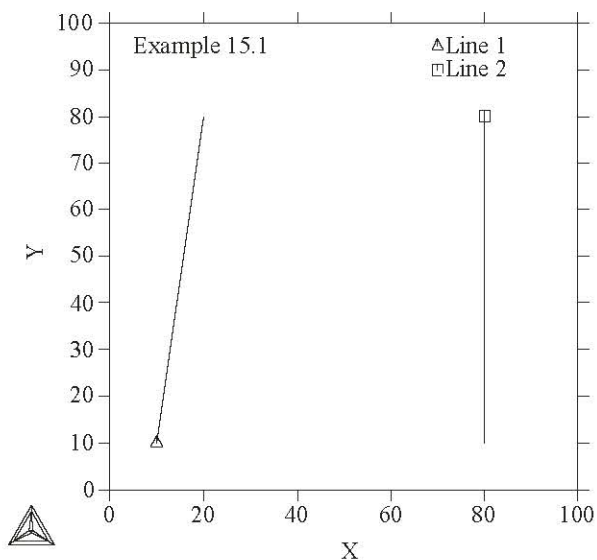
TITLEEXAMPLE 1 XTEXT X
YTEXTY

DATASET 1 Two lines started with two symbols
ATTRIBUTE CENTER

0.050.95 N'Example 1
0.70.95 NS'Line 1
0.70.90 NS2'Line 2 1010S1
2080D
8080S2
8010D
5060

```

THERMO-CALC (2001.08.16:11.26): EXAMPLE 15.1



---

## Example 2 – Draw Polygons and Symbols

```
$DATAPLOT Example 2

PROLOG 2 EXAMPLE 20<X<100, 0<Y<100

XSCALE0.00000100

YSCALE0.00000100

XTYPE LINEAR YTYPE LINEAR

XLENGTH11.5000

YLENGTH11.5000

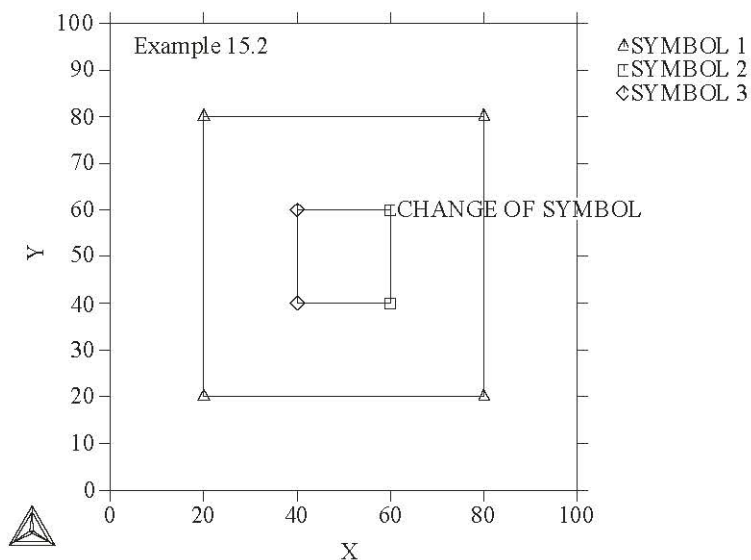
TITLEEXAMPLE 2 XTEXT X
YTEXTY


DATASET 2 Two ploygons with three types of symbols ATTRIBUTE CENTER
CLIP OFF

0.050.95 N'Example 2
1.10.95 NS1'SYMBOL 1
1.10.90 NS2'SYMBOL 2
1.10.85 NS3'SYMBOL 3

BLOCK X=C1; Y=C2; GOC=C3,DSWA
4040M
4060
6060S2'CHANGE OF SYMBOL
6040
4040S0
BLOCKEND

BLOCK X=C1*100; Y=C2*100; GOC=C3,DSWA 0.20.2 MS1
0.20.8
0.80.8
0.80.2
0.20.2
BLOCKEND
```



### Example 3 – Using Strings and Various Line Types

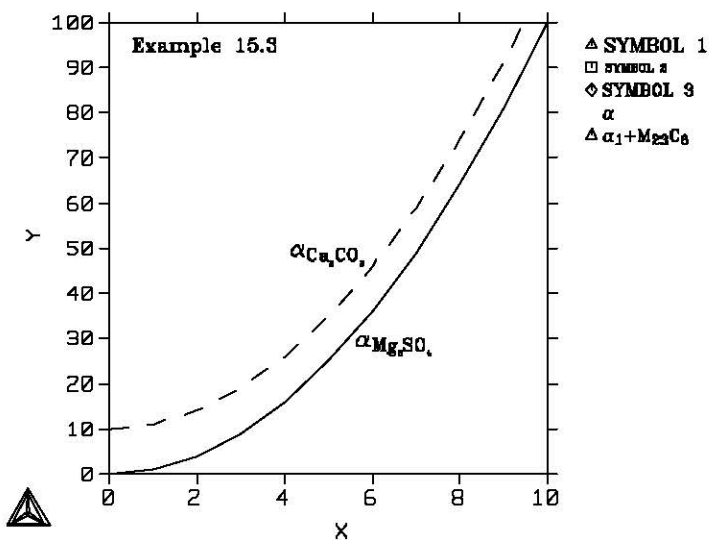
```
$DATAPLOT Example 3
PROLOG 3 EXAMPLE 3 0<X<10, 0<Y<100
XSCALE0.0000010
YSCALE0.00000100
XTYPE LINEAR
YTYPE LINEAR
XLENGTH11.5000
YLENGTH11.5000
TITLE EXAMPLE 3 XTEXT X
YTEXT Y
DATASET 3 Draw curves; plot formatted texts and symbols
$Define some strings: STRING BCC ^Ga^F0
STRING BCC1 ^Ga^F0^D0^S8,1^S0^U0
STRING M23C6 M^D0^S8,23^S0^U0C^D0^S8,6^S0^U0
STRING ACA2CO3 ^Ga^F0^D0^S8Ca^D0^S4,2^S0^U0^S8CO^D0^S4,3^S0^U0 STRING AMG2SO4
^Ga^F0^D0^S8Mg^D0^S4,2^S0^U0^S8SO^D0^S4,4^S0^U0
$ Note: if as PostScript output:
$STRING BCC !a
$STRING BCC1 !a^do1$
$STRING M23C6 M^do23$C^do6$
$STRING ACA2CO3 !a^doCa^do2$^doCO^do3$
$STRING AMG2SO4 !a^doMg^do2$^doSO^do4$ ATTRIBUTE CENTER
```

```

CLIP OFF FONT 2
0.05 0.95 N'Example 3
1.10.95 NS1'SYMBOL 1 CHARSIZE 0.2
1.10.90 NS2' SYMBOL 2 CHARSIZE 0.3
1.10.85 NS3'SYMBOL 3 1.10.80 N' ~BCC
1.10.75 NS1'~BCC1+~M23C6
SYMBOLSIZE 0.4
CHARSIZE 0.4
0.41 0.50 N'~ACA2CO3
0.56 0.30 N'~AMG2SO4 CLIP ON
LINETYPE 1
BLOCK X=C1; Y=C1*C1; GOC=C2, DWA
1 2 3 4 5 6 7 8 9 10
BLOCKEND LINETYPE 2
BLOCK X=C1; Y=C1*C1+10; GOC=C2, DWA
0 M 1 2 3 4 5 6 7 8 9 10
BLOCKEND
0 M

```

THERMO-CALC (2001.08.16:13.44) : EXAMPLE 15.3



## Example 4 – Draw Curves Defined by Functions

```

$DATAPLOT Example 4
PROLOG 4 EXAMPLE 40<X<100, 0<Y<100

```

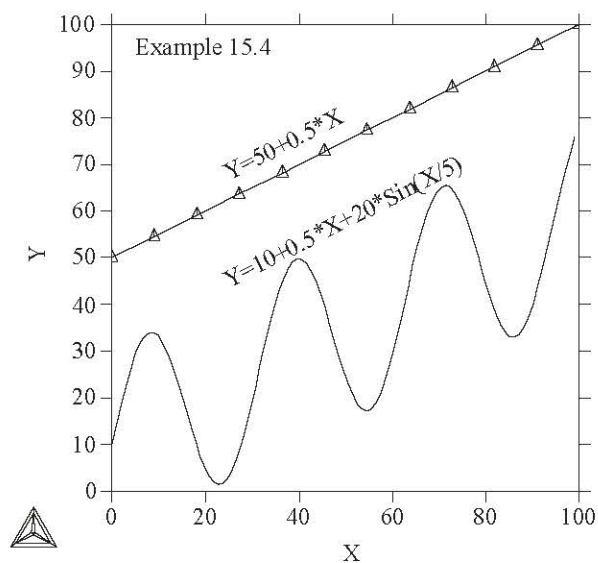


```

XSCALE0.00000100
YSCALE0.00000100
XTYPE LINEAR YTYPE LINEAR
XLENGTH11.5000
YLENGTH11.5000
TITLEEXAMPLE 4 XTEXT X
YTEXTY
DATASET 4 Plot two functions as lines: ATTRIBUTE CENTER
0.050.95 N'Example 4
$ Draw two lines defined by FUNCTIONS:
FUNCTION Y=10+0.5*X+20*Sin(X/5); 0 100 100; DWA;
FUNCTION Y=50+0.5*X; 0 100 10; DS1WA;
$ Write funtions beside the lines:
$Note the real rotation angle (27 degree) can be seen
$only on the PostScript hardcopy! 0.250.68 N'^RO27Y=50+0.5*X
0.250.45 N'^RO27Y=10+0.5*X+20*Sin(X/5)

```

THERMO-CALC (2001.08.16:16.32): EXAMPLE 15.4



## Example 5 – Use Included Files for Predefined Symbols

```

$DATAPLOT Example 5
PROLOG 5 EXAMPLE 50<X<100, 0<Y<100
XSCALE0.00000100
YSCALE0.00000100

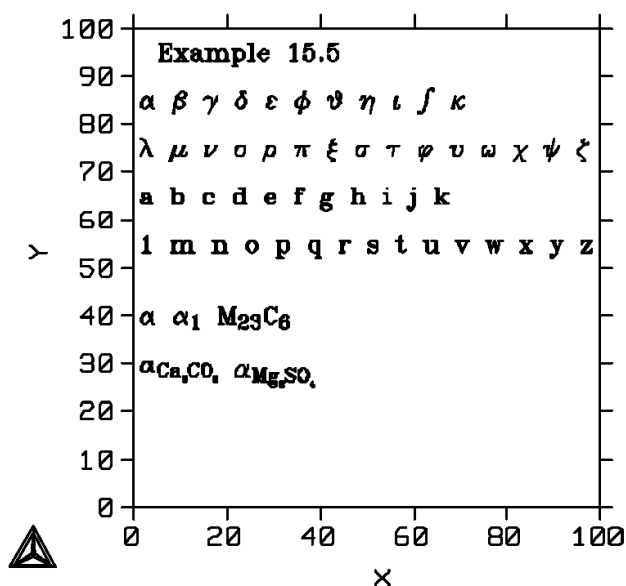
```

```

XTYPE LINEAR YTYPE LINEAR
XLENGTH11.5000
YLENGTH11.5000
TITLEEXAMPLE 5 XTEXT X
YTEXTY
DATASET 5 Write characters in various fonts, and defined symbols FONT 2
INCLUDE <DATAPLOT-EXAMPLE-PATH>INCLUDE.EXP ATTRIBUTE CENTER
0.050.95 N'Example 5 CLIP OFF
0.010.85 N'~TEST1A
0.010.75 N'~TEST1B
0.010.65 N'~TEST2A
0.010.55 N'~TEST2B
0.010.40 N'~BCC ~BCC1 ~M23C6
0.010.30 N'~ACA2CO3 ~AMG2SO4

```

THERMO-CALC (2001.08.16:17.06) : EXAMPLE 15.5



The INCLUDE.EXP file has the following content:

```

STRING TEST1A ^Ga b c d e f g h i j k^F0
STRING TEST1B ^Gl m n o p q r s t u v w x y z^F0 STRING TEST2Aa b c d e f g h i j k
STRING TEST2B l m n o p q r s t u v w x y z STRING BCC ^Ga^F0
STRING BCC1 ^Ga^F0^D0^S8,1^S0^U0
STRING BCC2 ^Ga^F0^D0^S8,2^S0^U0 STRING FCC ^Gc^F0

```

---

```

STRING FCC1 ^Gc^F0^D0^S8,1^S0^U0 STRING FCC2 ^Gc^F0^D0^S8,2^S0^U0

STRING L Liquid STRING SIGMA ^Gs^F0 STRING MU ^Gm^F0 STRING LAVES ^G1^F0 STRING CHI
^Gx^F0 STRING KSI ^Gr^F0

STRING MCETA ^S12^Gh^F0^S0 STRING M2CM^D0^S8,2^S0^U0C STRING M2CT M^D0^S10,2^S0^U0C
STRING M6CM^D0^S8,6^S0^U0C

STRING M23C6 M^D0^S8,23^S0^U0C^D0^S8,6^S0^U0 STRING M7C3
M^D0^S8,7^S0^U0C^D0^S8,3^S0^U0 STRING M3C2 M^D0^S8,3^S0^U0C^D0^S8,2^S0^U0 STRING MC1-X
MC^D0^S8,1-x^S0^U0

STRING XC x^D0^S7,C^S0^U0 STRING XFE x^D0^S7,Fe^S0^U0 STRING XMO x^D0^S7,Mn^S0^U0
STRING XW x^D0^S7,W^S0^U0 STRING UW ~XW/(~XMO+~XW)

STRING ac a^D0^S7,C^S0^U0 STRING ACC a^D0^S7,C^S0^U0

STRING ACA2CO3 ^Ga^F0^D0^S8Ca^D0^S4,2^S0^U0^S8CO^D0^S4,3^S0^U0 STRING AMG2SO4
^Ga^F0^D0^S8Mg^D0^S4,2^S0^U0^S8SO^D0^S4,4^S0^U0

$ Note: if as PostScript output:

$STRING TEST1A !a !b !c !d !e !f !g !h !i !j !k^fo27

$STRING TEST1B !l !m !n !o !p !q !r !s !t !u !v !w !x !y !z^fo27

$STRING TEST2Aa b c d e f g h i j k

$STRING TEST2B1 m n o p q r s t u v w x y z

$STRING BCC !a

$STRING BCC1 !a^do1$

$STRING BCC2 !a^do2$

$STRING FCC !c

$STRING FCC1 !c^do1$

$STRING FCC2 !c^do2$

$STRING L Liquid

$STRING SIGMA !s

$STRING MU !m

$STRING LAVES !l

$STRING CHI !x

$STRING KSI !r

$STRING MCETA !h

$STRING M2CM^do2$C

$STRING M2CT M^do2$C

$STRING M6CM^do6$C

$STRING M23C6 M^do23$C^do6$

$STRING M7C3 M^do7$C^do3$

$STRING M3C2 M^do3$C^do2$

$STRING MC1-X MC^do1-x$

```

---

```

$STRING XC x^doC$
$STRING XFE x^doFe$
$STRING XMO x^doMo$
$STRING XW x^doW$
$STRING UW ~XW/ (~XMO+~XW)
$STRING ac a^doC$
$STRING ACC a^doC$
$STRING ACA2CO3 !a^doCa^do2$^doCO^do3$
$STRING AMG2SO4 !a^doMg^do2$^doSO^do4$

```

## Example 6 – Plot Triangular Diagrams for Ternary Systems

```

$DATAPLOT Example 6
PROLOG 6 EXAMPLE 6 0<X<0.969224, 0<Y<1.00000
XSCALE0.000000.969224
YSCALE0.307492E-011.00000
XTYPE LINEAR YTYPE LINEAR
XLENGTH11.5000
YLENGTH11.5000 TITLE A-B-C at T=1000 K XTEXT MOLE_FRACTION B YTEXT MOLE_FRACTION C
DIAGRAM_TYPE TRIANGULAR YES YES
DATASET 6 Plot a ternary phase diagram CLIP OFF
0.70 0.95 N'Example 6 0.85 0.30 N'B2C
0.54 0.87 N'Diamond CHARSIZE 0.25
1.4E+01 1.10E+01 MVA'1:*B2C Liquid
1.4E+01 1.05E+01 MVA'2:*Diamond Liquid
0.10 0.10 N'Liquid
0.48 0.45 N'Diamond+
0.48 0.40 N' B2C+Liquid 5.80E-01 5.40E-02 MWA' 1
1.90E-01 2.40E-01 MWA' 1
0.65E-01 2.50E-01 MWA' 2
CHARSIZE 0.45
-0.10 -0.05 N'A
1.06 -0.05 N'B
0.500.95 N'C
CHARSIZE 0.35
$$ Calculated A-B-C Phase Equilibrium Data:
$ PHASE REGION FOR:
$F0 LIQUID

```

```
$E DIAMOND_A4
$F0 B2C
$ INVARIANT EQUILIBRIUM COLOR2
BLOCK X=C1; Y=C2;GOC=C3,WAD; 2.4555855989E-013.5568857193E-01M
0.0000000000E+009.9999523163E-01
2.4555855989E-013.5568857193E-01M
6.6666668653E-013.3333334327E-01
0.0000000000E+009.9999523163E-01M
6.6666668653E-013.3333334327E-01 COLOR1
BLOCKEND
$ PHASE REGION FOR:
$E LIQUID
$F0 B2C
BLOCK X=C1; Y=C2;GOC=C3,WAD;
$ PLOTTED COLUMNS ARE : X(LIQUID,B) and X(LIQUID,C)
2.2030337155E-011.2340000272E-01M
2.2632879019E-011.1058768630E-01
2.3371633887E-019.9345825613E-02
2.4253317714E-018.9345827699E-02
2.6429468393E-017.2744041681E-02
2.8429466486E-016.2814079225E-02
2.9617273808E-015.8319382370E-02
3.2811737061E-014.9470417202E-02
3.6353862286E-014.3130427599E-02
3.9895987511E-013.8979098201E-02
4.5209178329E-013.5266116261E-02
5.2293431759E-013.3152002841E-02
6.1148744822E-013.3077053726E-02
6.4690870047E-013.3490389585E-02
6.8232995272E-013.4017231315E-02
7.3546189070E-013.4814555198E-02
7.5317251682E-013.5033416003E-02
8.0630439520E-013.5373892635E-02
8.5943627357E-013.4983776510E-02
9.1256815195E-013.3575300127E-02
9.6747112274E-013.0857827514E-02
```

---

```

9.6922445297E-013.0749246478E-02
2.2030337155E-011.2340000272E-01M
2.1294665337E-011.5308913589E-01
2.1171525121E-011.8851040304E-01
2.1532440186E-012.2393165529E-01
2.2180187702E-012.5935292244E-01
2.2992117703E-012.9477417469E-01
2.3888295889E-013.3019542694E-01
2.4555855989E-013.5568857193E-01
$ PLOTTED COLUMNS ARE : X(B2C,B) and X(B2C,C) 6.6666668653E-013.3333334327E-01M
6.6666668653E-013.3333334327E-01
$ TIELINES COLOR3
6.6666668653E-013.3333334327E-01M
8.7775242329E-013.4625384957E-02
6.6666668653E-013.3333334327E-01M
7.9250496626E-013.5342670977E-02
6.6666668653E-013.3333334327E-01M
2.4555824697E-013.5568737984E-01
6.6666668653E-013.3333334327E-01M
2.3944084346E-019.2542596161E-02
6.6666668653E-013.3333334327E-01M
2.3359020054E-013.0954307318E-01
6.6666668653E-013.3333334327E-01M
2.2585247457E-012.7766343951E-01
6.6666668653E-013.3333334327E-01M
2.1618695557E-011.3621240854E-01
2.2632879019E-011.1058768630E-01M
6.6666668653E-013.3333334327E-01 COLOR1
BLOCKEND
$ PHASE REGION FOR:
$F0 DIAMOND_A4
$E B2C
BLOCK X=C1; Y=C2;GOC=C3,WAD;
$ PLOTTED COLUMNS ARE : X(DIAMOND_A4,B) and X(DIAMOND_A4,C)
0.0000000000E+009.9999523163E-01M
0.0000000000E+009.9999976158E-01 BLOCKEND

```

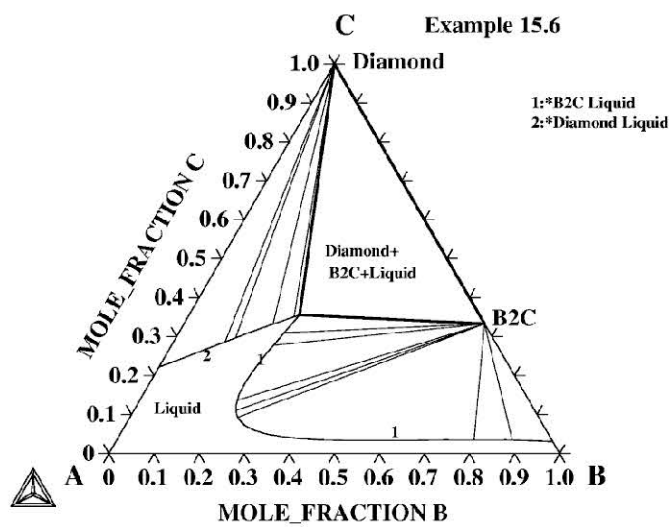
---

```

$ PHASE REGION FOR:
$E LIQUID
$F0 DIAMOND_A4
BLOCK X=C1; Y=C2;GOC=C3,WAD;
$ PLOTTED COLUMNS ARE : X(LIQUID,B) and X(LIQUID,C)
2.45558E-01  3.55688E-01 M
2.02635E-01  3.34830E-01
1.62439E-01  3.13753E-01
1.22439E-01  2.91531E-01
8.24390E-02  2.68542E-01
4.24390E-02  2.45480E-01
2.43905E-03  2.23138E-01
2.49999E-07  2.21816E-01
$ TIELINES COLOR3
0.00000E+00  9.99995E-01 M
2.35291E-01  3.50859E-01
0.00000E+00  9.99994E-01 M
1.98265E-01  3.32609E-01
0.00000E+00  9.99994E-01 M
1.32400E-01  2.97160E-01
0.00000E+00  9.99993E-01 M
1.14399E-01  2.86953E-01 BLOCKEND

```

**THERMO-CALC (2001.08.24:09.50) : A-B-C at T=1000 K**



---

## Example 7 – Color Codes and Effects

```
$DATAPLOT Color Codes & Color Effects
PROLOG 10 Color Codes  0<X<1.0, 0<Y<1.0
XSCALE0.01.0
YSCALE0.01.0
XTYPE LINEAR
YTYPE LINEAR
XLENGTH11.5000
YLENGTH11.5000
TITLE Color Outputs XTEXT Color Codes YTEXT  Color Effects
DATASET 10 Various Color Codes for Color Outputs: CHARSIZE 0.3
LINETYPE 1
BLOCK X=C1; Y=C2;GOC=C3,WAD;
0.05  0.95 MNA'Color Code: Color Effect
0.55 0.95 MNA'Color Code: Color Effect CHARSIZE 0.25
COLOR 1
0.05 0.88 MNA'1: Black CLIP ON
0.22  0.88 M
0.45 0.88
CLIP OFF COLOR 2
0.05 0.82 MNA'2: Red CLIP ON
0.22  0.82 M
0.45 0.82
CLIP OFF COLOR 3
0.05 0.76 MNA'3: Green CLIP ON
0.22  0.76 M
0.45 0.76
CLIP OFF COLOR 4
0.05 0.70 MNA'4: Blue CLIP ON
0.22  0.70 M
0.45 0.70
CLIP OFF COLOR 5
0.05 0.64 MNA'5: Yellow CLIP ON
0.22  0.64 M
0.45 0.64
CLIP OFF COLOR 6
```

---



---

0.05 0.58 MNA'6: Magenta CLIP ON  
0.22 0.58 M  
0.45 0.58  
CLIP OFF COLOR 7  
0.05 0.52 MNA'7: Cyan CLIP ON  
0.22 0.52 M  
0.45 0.52  
CLIP OFF COLOR 8  
0.05 0.46 MNA'8: Purple CLIP ON  
0.22 0.46 M  
0.45 0.46  
CLIP OFF COLOR 9  
0.05 0.40 MNA'9: Gold CLIP ON  
0.22 0.40 M  
0.45 0.40  
CLIP OFF COLOR 10  
0.05 0.34 MNA'10: Turquoise CLIP ON  
0.22 0.34 M  
0.45 0.34  
CLIP OFF COLOR 11  
0.05 0.28 MNA'11: Pink CLIP ON  
0.22 0.28 M  
0.45 0.28  
CLIP OFF COLOR 12  
0.05 0.22 MNA'12: Gray CLIP ON  
0.22 0.22 M  
0.45 0.22  
CLIP OFF COLOR 13  
0.05 0.16 MNA'13: Orangered CLIP ON  
0.22 0.16 M  
0.45 0.16  
CLIP OFF COLOR 14  
0.05 0.10 MNA'14: Moroon CLIP ON  
0.22 0.10 M  
0.45 0.10  
CLIP OFF COLOR 15

---

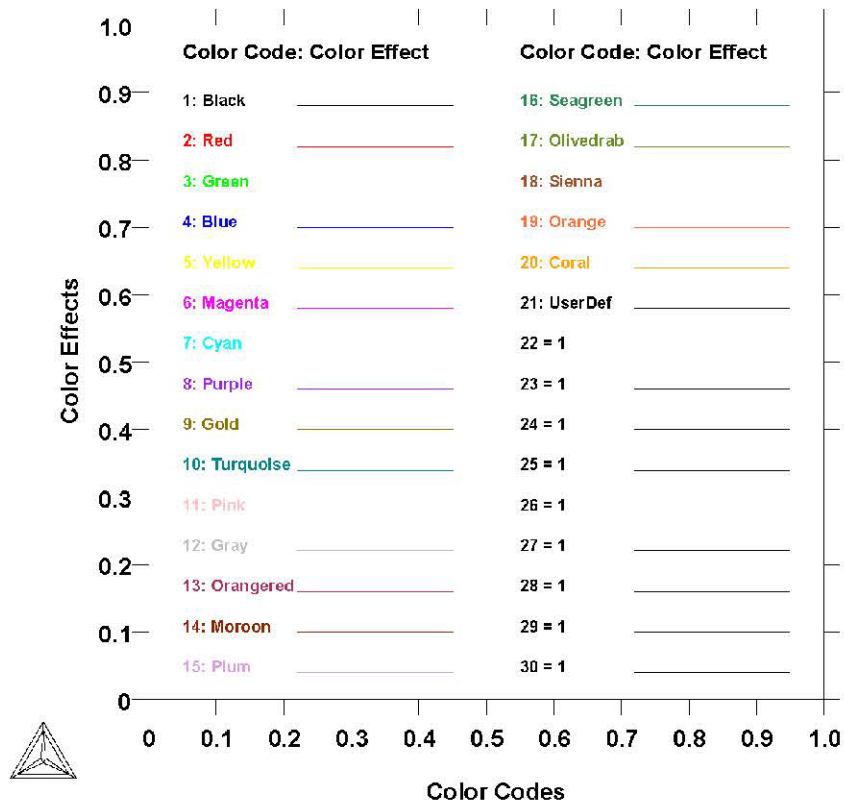
---

```
0.05 0.04 MNA'15: Plum CLIP ON
0.22 0.04 M
0.45 0.04
CLIP OFF COLOR 16
0.55 0.88 MNA'16: Seagreen CLIP ON
0.72 0.88 M
0.95 0.88
CLIP OFF COLOR 17
0.55 0.82 MNA'17: Olivedrab CLIP ON
0.72 0.82 M
0.95 0.82
CLIP OFF COLOR 18
0.55 0.76 MNA'18: Sienna CLIP ON
0.72 0.76 M
0.95 0.76
CLIP OFF COLOR 19
0.55 0.70 MNA'19: Orange CLIP ON
0.72 0.70 M
0.95 0.70
CLIP OFF COLOR 20
0.55 0.64 MNA'20: Coral CLIP ON
0.72 0.64 M
0.95 0.64
CLIP OFF COLOR 21
0.55 0.58 MNA'21: UserDef CLIP ON
0.72 0.58 M
0.95 0.58
CLIP OFF COLOR 22
0.55 0.52 MNA'22 = 1 CLIP ON
0.72 0.52 M
0.95 0.52
CLIP OFF COLOR 23
0.55 0.46 MNA'23 = 1 CLIP ON
0.72 0.46 M
0.95 0.46
CLIP OFF
```

---

BLOCKEND

## THERMO-CALC (2012.06.18:14.01) : Color Outputs



# Database Manager User Guide

Version 2016a



---

# Introduction to the Database Manager Guide

In this section:

---

<i>Thermodynamic and Kinetic/Mobility Databases</i> .....	3
<i>Initialization of the DATA Module</i> .....	3
<i>Initiation Parameter Examples</i> .....	4

## Thermodynamic and Kinetic/Mobility Databases

This guide describes how to define and construct a thermodynamic or kinetic database. It includes details about the data structures and formats of the Thermo-Calc databases as well as the Diffusion Module (DICTRA) database-extensions.

The Thermo-Calc databases are created and maintained in the Thermo-Calc Database Format (TDB) which is an international standard for the CALPHAD-type thermodynamic calculations and kinetic simulations. This document gives a full description of the TDB format (with the Diffusion Module (DICTRA) database extension) and is a comprehensive guide about how to create and manage a Thermo-Calc (and Diffusion Module (DICTRA)) database.

Usually, a Thermo-Calc or Diffusion Module (DICTRA) database is constructed as a single text file with an extension of TDB, for example, `PAQS2setup.TDB`. For some databases (especially large databases used with older versions of Thermo-Calc or Diffusion Module (DICTRA)) a database may consist of one primary-definition file (`***setup.TDB`) and several additional-definition TDB files (such as `***param.TDB`, `***funct.TDB`, `***refer.TDB`, etc. These are built for a variety of defined parameters, functions, references and so forth, and are linked to the `***setup.TDB` file through the correct use of the [TYPE\\_DEFINITION](#) on page 18 and/or [FTP\\_FILE](#) on page 21 commands inside the `***setup.TDB` file.



With Thermo-Calc, Precipitation Module (TC-PRISMA) and Thermo-Calc Software Development Kits (SDKs), you can code everything into a single **\*\*\*setup.TDB** file for a database at any scale.

## Initialization of the DATA Module

The following explains how a database initiation file (or a database directory file) is constructed to work with the DATA module. When you start, DATA looks for this file that has information about the available predefined databases.

The *database initiation file* is called:

- Windows: `TC_INITD.TDB` (or `TC_INITD`)
- Linux/UNIX: `initd.tdb`

You can have your own file, but it is more efficient to define an environment variable with the default name as above, and then during installation, translate it to a common initiation file name. The common file is automatically copied by the Thermo-Calc installation script to the following directories:

- Windows: `\DATA\` under the directory defined by the `TCPATH` parameter
- Linux/UNIX: `/data/` under the directory defined by the `TC_DATA` parameter.

The database manager can find the file on a local computer (independent installations) or a connected server (server installations).

When editing or modifying the definitions of initiation parameters (including short-names, paths and subdirectories, database definition file names, and instructive database descriptions) for the available databases in the database initiation file a specific format is used with the fields:

- The first field gives the abbreviated name for the database (to a maximum of five characters)
- The second field specifies a path and filename (maximum 78 characters) containing the database path definition and the actual database definition (*setup*) file name, where the extension is either `TDB` (which stands for original textual TDB file) or `TDC` (which is encrypted from the original TDB file). There are differences between platforms with respect to entering parameters as listed in the table.
- The third field (maximum 60 characters) details an optional full name (and version/subversion numbers) for the brief database description.

## Initiation Parameter Examples

Parameter	Windows	Linux/Unix
The <i>setup</i> file name must consist of a main part and an extension of a maximum of three characters:	For example, <code>SSOL5SETUP.TDB</code>	For example, <code>ssol5setup.tdb</code>
Database path definition	Use a back-slash \	Use a forward-slash /
All databases should be normally located in subdirectories that are under the directory defined by the:	<code>TCPATH</code> parameter or under its subdirectory <code>\DATA\</code>	<code>TC_DATA</code> parameter or under its subdirectory <code>/data/</code>



Each entry record (i.e. for a single database) must finish with an exclamation mark !. There should be no spaces or commas within the first and second fields since these characters are taken as field separators, while spaces or commas can be used in the third field.

You can write each database entry on one or two lines (up to the!), it is recommended that the third field is added as follows:

- Windows: on the same line as the first and second fields.
- Linux/UNIX: on the following line.

The following are examples of an initiation file defining two databases named SSOL6 and TCFE8.

## Windows

```
SSOL6 TCPATH\DATA\SSOL6\SSOL6SETUP.TDC  SGTE Solutions Database  
version 6.0 !
```

```
TCFE8 TCPATH\DATA\TCFE8\TCFE8SETUP.TDC  TCS Steels/Fe-Alloys Database  
version 8.0 !
```

## Linux/UNIX

```
ssol5 TC_DATA/data/ssol5/ssol5setup.tdc  
      SGTE Solutions Database version 5.1  !  
Tcfe8 TC_DATA/data/tcfe8/tcfe8setup.tdc  
      TCS Steels/Fe-Alloys Database version 8.0 !
```



# The Database Definition File and Keywords

In this section:

---

<i>Database Definition File Syntax</i> .....	7
<i>ELEMENT</i> .....	7
<i>SPECIES</i> .....	8
<i>PHASE</i> .....	9
<i>CONSTITUENT</i> .....	14
<i>ADD_CONSTITUENT</i> .....	15
<i>COMPOUND_PHASE</i> .....	16
<i>ALLOTROPIC_PHASE</i> .....	16
<i>TEMPERATURE_LIMITS</i> .....	16
<i>DEFINE_SYSTEM_DEFAULT</i> .....	16
<i>DEFAULT_COMMAND</i> .....	17
<i>DATABASE_INFORMATION</i> .....	18
<i>TYPE_DEFINITION</i> .....	18
<i>FTP_FILE</i> .....	21
<i>FUNCTION</i> .....	22
<i>PARAMETER</i> .....	24
<i>GIBBS Parameter Name</i> .....	26
<i>OPTIONS</i> .....	31
<i>TABLE</i> .....	32
<i>ASSESSED_SYSTEMS</i> .....	32
<i>REFERENCE_FILE</i> .....	35
<i>LIST_OF_REFERENCE</i> .....	36
<i>CASE and ENDCASE</i> .....	38
<i>VERSION_DATA</i> .....	39

---

## Database Definition File Syntax

The database definition (\*.TDB) file (normally named `***setup.TDB`) consists of a set of keyword codes each followed by one or several parameters (arguments).

- A complete keyword entry must end with an exclamation mark (!).
- A single keyword entry can be up to 2000 characters long. However, the maximum length of a line in an \*.TDB file is 78 characters--it may be necessary to continue the keyword parameter (arguments) on several lines. The ! must be at the end of the last line.
- It is recommended to always have at least one empty space at the beginning of each continuation line for the keyword parameters (arguments); otherwise, the DATA module can misunderstand the parameters (or arguments), or issue an error message.
- The keyword and its various parameters (arguments) are separated by a space or a comma.
- A dollar sign (\$) in the first position of the line indicates that the line is a comment line, which is ignored by the DATA module.

When the database is selected the DATA module only reads the database definition file (`***setup.TDB`) once, from beginning to end. The DATA module checks continuously when reading the definition file. This implies that (nearly) everything must be declared or defined before it is used in any other way.

For example, if the GRAPHITE phase is to be included in the database definition, the element C (carbon) and the phase GRAPHITE must be defined before declaring that carbon dissolves in graphite. This definition order is necessary to build the internal data structure acceptable by the DATA module (during its consistency checking).

This topic gives a description of the available keywords and the appropriate arguments. A basic knowledge of the Gibbs Energy System (GIBBS) module is assumed.

This syntax is used:

```
KEYWORD [arg.1]*# [arg.2]*## {optional arg.3}!
```

The keywords are written in full length but can be abbreviated as long as the abbreviation is unique. A keyword may have syntax consisting of several arguments and optional arguments. The number, # or ##, in the notation, [...]\*# or [...]\*##, indicates an argument with a maximum length of # ASCII characters.



Arguments within square brackets [...] must always be given, but are optional when enclosed in curly brackets {...}.

## ELEMENT

```
ELEMENT [element name]*2 [ref. state]*24 [mass] [H298] [S298] !
```

The *element name* (maximum two characters) is the one found in the periodic chart but there are no naming restrictions. However, the GIBBS module only recognizes UPPER-case element names (if the Upper Case Mode is selected by the GIBBS command [REINITIATE on page 83](#)), which means that lower-case (if defined in a database) is automatically converted to UPPER-case by the DATA/GIBBS module.

The elements are automatically entered as species using the same names of the elements. If, for example, the species corresponding to FE needs to be named FE1, you can define the species as FE1, which results in an element named FE and a species named FE1. Vacancies (VA) and electrons (denoted either as /- in gaseous, liquid or solid phases, or ZE in an aqueous solution phase), need to be entered as special elements for correct handling by the DATA module.

The *reference (ref.) state* (maximum 24 characters) is the stable phase (at 298.15 K and 1 bar) that should contain this element and be used as the reference state for all element thermodynamic data. The *mass*, given in gram per mole, is used in various calculation programs and should always be given the correct value. *H298* and *S298* denote the enthalpy and entropy difference between 0 and 298.15 K for the element in SI units. If these are unknown, the values can be set to zero. All this information (reference state, H298 and S298) define the SER (Stable Element Reference state).

## Examples

```

ELEMENT /- ELECTRON_GAS      0.0  0.0  0.0  !
ELEMENT VA VACUUM            0.0  0.0  0.0  !
ELEMENT ZE UNIT_CHARGE       0.0000000001  0.0  0.0  !
ELEMENT AL FCC_A1            26.98154  4577.296  28.3215  !
ELEMENT C GRAPHITE           12.011  1054.0    5.74  !
ELEMENT FE BCC_A2            55.847  4489    27.28  !
ELEMENT O 1/2_MOLE_O2 (G)    15.9994  4341    102.5158  !
ELEMENT TI HCP_A3            47.88  4810    30.648  !
ELEMENT ZR HCP_A3            91.224  5566.27  39.181  !
ELEMENT ZY DUMMY             1        1        1  !

```

## SPECIES

```
SPECIES [species name]*24 [stoichiometric formula] !
```

This keyword defines species in the data structure. Every *species name* (maximum 24 characters) must be unique. The species are built from the predefined set of elements in the stoichiometric formula. If an undefined element is referenced, DATA displays an error message and the data structure is probably damaged.

The species names do not have to be the same as the stoichiometry formula, although in general this is recommended. The elements are automatically entered as species using the same names of the elements.



You can define a species name as a mixture of UPPER-case and lower-case letters in a database, but the DATA module automatically converts all lower-case to UPPER-case because the GIBBS module only recognizes UPPER-case species names.

When naming the species in a database, use special characters (such as +, -, \_ / and .) in species names. Avoid using other special characters (such as ( and ) ).

The *stoichiometric formula* is written with a simplified chemical notation, in which the chemical elements should always be given in UPPER-case and in any preferred order, and the stoichiometric coefficients are written in either real numerical factors or integer digits.



It is important that the numerical factor of 1 is not left out. Subgroups are not allowed in a stoichiometry formula; however, while specifying the stoichiometry formula for a specific species in a database, you can specify it in a way that some elements (always together with the corresponding partial stoichiometric coefficients) are repeated (as in the examples below).

## Examples

```
SPECIES AL2O3      AL2O3 !
SPECIES Silica     SI1O2 !
SPECIES NaSb_6OH   NA1SB1O6H6 !
SPECIES FE+2       FE/+2 !
SPECIES SB-3       SB/-3 !
SPECIES AlCl2/3     AL.33333CL.666667 !
SPECIES AL1CL1H2O2  AL1CL1H2O2 !
SPECIES AlCl3_3H2O  AL1CL3H6O3 !
SPECIES AlO2H2Cl.H6O3 AL1O2H2CL1H6O3 !
SPECIES AlCl2-OH.3H2O AL1CL2O1H1H6O3 !
SPECIES AlCl2OH.3Water AL1O1H1CL2H6O3 !
```

## PHASE

```
PHASE [phase name]*24 [data-type code]*8 [numb. subl.] [sites in
subl. 1] [sites in subl. 2] etc... {auxiliary text string} !
```

This keyword defines a phase and its properties (except for what species are allowed to enter it and for its parameters).

The *phase name* (maximum 24 characters) must be unique; otherwise the DATA module sees it as an attempt to redefine a previously defined phase. This causes DATA to display an error message and ignore

the rest of the line. A phase name can be suffixed by an underscore ( \_ ) and letters to identify the physical state(s) or structure type(s) of the phase.

### Examples of Recommended Suffixes

Suffix	Definition
ABC_S	The ABC phase in solid state.
ABC_S2	The ABC phase in solid state 2.
ABC_S3	The ABC phase in solid state 3.
ABC_LT	The ABC phase in solid state at low temperatures.
ABC_HT	The ABC phase in solid state at high temperatures.
ABC_L	The ABC phase in liquid state.
ABC_LIQ	The ABC phase in liquid state.
FCC_A1	The FCC phase in disordered structure type A1.
FCC_L12	The FCC phase in ordered structure type L12.

The *phase name* can also be attached with a colon sign ( : ) and a letter for a legal GIBBS phase-type code (e.g. IONIC\_LIQ:Y and GAS:G).

### GIBBS Phase-type Codes

Code	Definition
G	Bit set for a gaseous mixture phase.
A	Bit set for an aqueous solution phase.
Y	Bit set for an ionic liquid solution phase (specially treated by the Ionic Two-Sublattice Liquid Model).
L	Bit set for a liquid solution phase (but not A (aqueous) or Y (ionic liquid)).
I	Bit set for a phase with charged species (but not G (gaseous), A (aqueous) or Y (ionic liquid)).
F	Bit set for an ordered FCC or HCP solution phase using the <i>Four Substitutional-Sublattice Ordering Model</i> (additionally, such a phase can also have interstitial sublattices).
B	Bit set for an ordered BCC solution phase using the <i>Four Substitutional-Sublattice Ordering Model</i> (additionally, such a phase can also have interstitial sublattices).



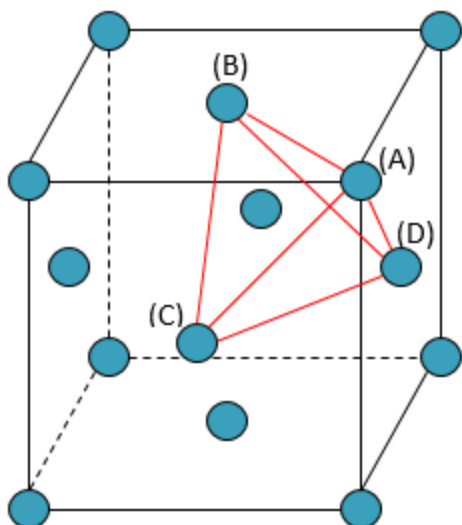
Other invalid characters (e.g.  $\mathbb{M}$  or  $\mathbb{P}$ ) are eventually treated, together with the colon (:), as a part of a phase name.

A  $\mathbb{G}$  phase (gaseous mixture) or an  $\mathbb{A}$  phase (aqueous solution) is usually treated as a substitutional phase without sublattice, and an  $\mathbb{L}$  phase (ordinary liquid solution) is normally (but not always) modelled as a substitutional phase without sublattice, too.

For ordered FCC or HCP phases, these four substitutional sublattices represent four corners of the regular tetrahedron on these lattices, all of which are the nearest neighbours, as shown.

### FCC Unit Cell Example

An FCC unit cell with the lattice positions indicated that correspond to the  $\mathbb{G}$  (FCC,A:B:C:D) end member. All lattice positions are equivalent for a four substitutional-sublattice ordering model.



A *Normal 4-Sublattice Model* requires that all the  $\mathbb{G}$  parameters for each of the end-members with the same elements but distributed on different sites be given separately. However, as these corners are identical lattice points, the phase-type option  $\mathbb{F}$  means that the  $\mathbb{G}$  parameters need be given only once. The possible permutations are handled automatically.

### Additional Clarification

An  $\mathbb{A}-\mathbb{B}$  binary solution phase (with the element  $\mathbb{A}$  located on one sublattice site and  $\mathbb{B}$  on the other three sublattice sites) treated by the Normal 4-Sublattice Model has to have four  $\mathbb{G}$  parameters for four end-members, i.e.

- $\mathbb{G}(\text{phase}, \mathbb{A}:\mathbb{B}:\mathbb{B}:\mathbb{B})$
- $\mathbb{G}(\text{phase}, \mathbb{B}:\mathbb{A}:\mathbb{B}:\mathbb{B})$

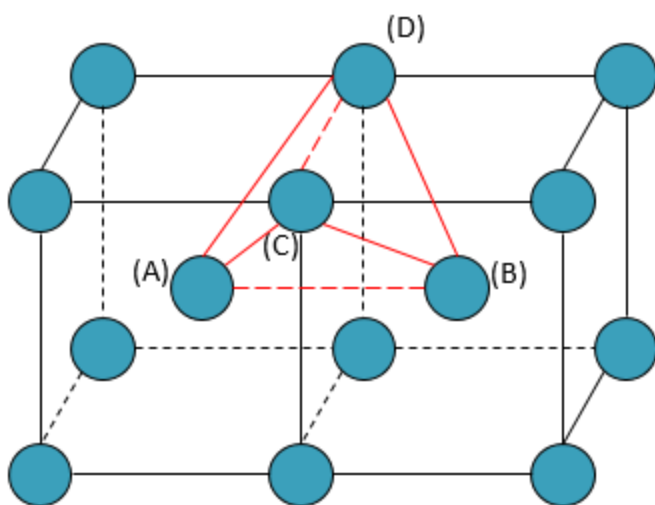
- $G(\text{phase}, B:B:A:B)$ , and
- $G(\text{phase}, B:B:B:A)$

This is because in the general case these  $G$  parameters can be different from each other. But for the FCC and HCP orderings, they are identical and thus all  $G$  parameters of such end-members need to be given only once, and the possible permutations are then automatically handled by the GIBBS module. Also, only one of the identical permutations is listed; in this example,  $G(\text{phase}, A:B:B:B)$  where it is alphabetically the first in the list of permutations. This significantly simplifies the usage of this model (*Four Substitutional-Sublattice Ordering Model*) in multicomponent alloys.

For ordered BCC phases, the phase-type option **B** means the same thing but it is more complicated since the 4-substitutional-sublattice ordering phase represents an irregular tetrahedron with two pairs of sites that are next nearest neighbours as shown:

### BCC Unit Cell Example

Two BCC unit cells with the lattice positions indicated that correspond to the  $G(\text{BCC}, A:B:C:D, 0)$  end member. Lattice positions (A) and (B) are equivalent, as are lattice positions (C) and (D) for a four substitutional-sublattice ordering model.



For an end member described by the parameter  $G(\text{phase}, A:B:C:D)$  A and B are next nearest neighbours, as are C and D. And the nearest neighbours of A (or B) are C and D. Thus, for an A-B binary solution phase (with the element A located on two sublattice sites and B on two sublattice sites) treated by the Normal 4-Sublattice Model, the end-member described by the  $G(\text{phase}, A:A:B:B)$  term has four nearest neighbour bonds between A and B atoms, whereas the end-member described by the  $G(\text{phase}, A:B:A:B)$  term has two nearest neighbour bonds between A and B atoms and three next nearest neighbour bonds.

The first end-member (described by the  $G(\text{phase}, A:A:B:B)$  term) represents B2-ordering and the second (described by the  $G(\text{phase}, A:B:A:B)$  term) stands for B32-ordering. There are two

permutations of the  $G(\text{phase}, A:A:B:B)$  term and four permutations of the  $G(\text{phase}, A:B:A:B)$  term, automatically conducted in the *Four Substitutional-Sublattice Ordering Model*. If you enter the unary, binary, ternary and quaternary parameters you are dealing with 1, 6, 21, 55 parameters for BCC:B, 1, 5, 15, 35 parameters for FCC:F and 1, 16, 81, 256 parameters for phases without F/B.

An additional feature with the phase-type options **F** and **B** is that a composition set that represents the solution phase has a suffix (indicating what ordering the phase has) that is automatically added to its phase name in some listings of equilibrium calculations (when performing either single-point or stepping or mapping calculations, and when plotting the calculated property diagrams or phase diagrams).

Such suffix indications can be:

Solution Phase	Suffix for Disordered Phase	Suffix for Ordered Phase
FCC PHASE	FCC_A1	FCC_L12
		FCC_L10
BCC PHASE	BCC_A2	BCC_B2
		BCC_B32
		BCC_D03
		BCC_L21
HCP PHASE	HCP_A3	HCP_D019
		HCP_B19



If you want to convert an existing database TDB-file to use the F/B feature, add the phase-type code to the corresponding phase name in the PHASE and CONSTITUENT commands in the TDB-file, then when running the LIST\_DATA command in the GES module. The created database file is in this less verbose format.

The *data-type code* consists of 1 to 8 characters where each character must stand for an action, which is to be coupled to this phase. The keyword [TYPE\\_DEFINITION](#) on page 18, described below, must be used in the current database to specify what action should be taken by DATA for each character code.

The data entries [numb. subl.] [sites in subl. 1] [sites in subl. 2] etc., specify the total number of sublattices (always as an integer digit) and the sites (i.e. stoichiometric coefficients) of each of the sublattices (given in either integer digits or real numerical factors) for the phase.

Optionally, an *auxiliary text string* (maximum 78 characters) can be given after the last [sites in sublattice #] but before the exclamation mark !. This string displays in connection with the phase name in some listings within the DATA module.

## Examples

```
PHASE GAS:G % 1 1.0 !
```



```

PHASE LIQUID:L %ZCDQ 2 1.0 1.0
> Metallic liquid solution, modelled by CEF Model. !
PHASE IONIC-LIQ:Y %ZCDQ 2 1.0 1.0
> Ionic liquid solution, modelled by Ionic Two-Sublattice Model. !
PHASE SPINEL:I %ZA 4 1 2 2 4
> Complex Spinel Solution, by CEF model with ionic constraints. !
PHASE M23C6 % 3 20.0 3.0 6.0 !
PHASE FCC_A1 %&A 2 1 1
> Disordered FCC phase; also as MX carbides/nitrides. !
PHASE FCC_L10 %&AX 3 0.75 0.25 1
> Ordered FCC phase, modelled by 2-Sublattice Model for Ordering. !
PHASE FCC_L12:F %&AX 5 0.25 0.25 0.25 0.25 1.0
> Ordered FCC phase, modelled by 4-Sublattice Model for Ordering. !
PHASE AQUEOUS:A %HIJMR 1 1.0
> Aqueous Solution: using the Complete Revised HKF Model. !

```

## CONSTITUENT

```
CONSTITUENT [phase name]*24 [constituent description]*2000 !
```

This keyword (and the [ADD\\_CONSTITUENT on the next page](#) keyword for large solution phase) defines the phase-constitution as a list of constituents (for a substitutional phase with no sublattice) or of constituent arrays (for a sublattice phase).

The *phase name* (maximum 24 characters) must be a predefined phase (i.e. already through the [PHASE on page 9](#) keyword).



It is important that if a phase bears a legal phase-type (among G, A, Y, L, I, F and B) in its phase definition (already by the PHASE keyword; such as GAS:G, SLAG:L, LIQUID:L, IONIC\_LIQ:Y, SPINEL:I, FCC\_L12:F, HCP\_D021:F, BCC\_B2:B, AQUEOUS:A), such a valid phase-type code must also always be attached to the phase name in the CONSTITUENT keyword (and the ADD\_CONSTITUENT keyword).



Specifying the phase name in UPPER-case is recommended. You can define a phase name as a mixture of UPPER-case and lower-case letters in a database, but the DATA module automatically converts all lower-case to UPPER-case because the GIBBS module only recognizes UPPER-case phase names.

The *constituent description* (maximum 2000 characters) is a list of the species that enter a phase. The list starts with a colon (:), indicating the start of the sub-list of species for the first sublattice, and different sublattices are separated by colons. The complete sequence ends with a final colon.

Optionally, each sublattice may specify which species are considered to be major constituents. This is done by adding a percent sign (%) directly to the species name. The start values on the site fractions of the major constituents should sum to 0.99 on a specific sublattice. Thus, the minor constituents (i.e. those without a %) add up to 0.01. A maximum of 2000 characters can be coded in the constituent description, continuing in sequent lines. If the phase has a constituent description longer than 2000 characters, the rest can be coded in one or several ADD\_CONSTITUENT keywords.

### Examples

```
CONSTITUENT BCC_A2 :FE
CONSTITUENT IONIC-LIQ:Y :FE+2 : SB-3: !
CONSTITUENT M23C6 :CR FE :FE CR W MO : C: !
CONSTITUENT AQUEOUS:A :H2O% AG+1 AGF AGCL AGCL2-1 AGI3-2 AGSO4-1
AGC2H4+1
    AGN2H6+1 AGC2N2-1 AGC2H4NO2 AL+3 ALF3 ALO2-1, ... : !
CONSTITUENT SPINEL:I : AL+3% CR+3 FE+2% FE+3 MG+2% NI+2
    : AL+3% CA+2 CR+3 FE+2 FE+3 MG+2% NI+2 VA
    : FE+2 MG+2 VA%
    : N-3 O-2% :!
```

## ADD\_CONSTITUENT

```
ADD_CONSTITUENT [phase name]*24 [constituent description]*2000 !
```

This keyword adds more constituents to a phase that already has some constituents. Its syntax is the same as for the [CONSTITUENT on the previous page](#) keyword. This keyword can be used several times, if the phase is very large, e.g. a gaseous mixture or a complex aqueous solution. This is useful when there are so many constituents in a phase that the 2000 characters available for the constituent description list is not enough.



Constituents are not necessary on all sublattices. In the second example below, no addition is made to the first sublattice.

### Examples

```
ADD_CONSTITUENT GAS :S1 S2 S3 ... : !
ADD_CONSTITUENT IM-PHASE : :CR:W ... : !
ADD_CONSTITUENT AQUEOUS:A :CUCL+1 CUCL2 CUCL2-1 CUCL3-2 CUOH+1 CUO2H2
CUO3H3-1
```

```
CUO4H4-2 CU2OH+3 CU2O2H2+2 CU3O4H4+2 NIO2H2 NIO3H3-1 NIO4H4-2
NI2OH+3
NI4O4H4+4 ZNOH+1 ZNO2H2 ZNO3H3-1 ZNO4H4-2 ... : !
```

## COMPOUND\_PHASE

```
COMPOUND_PHASE [phase name]*24 [data-type code]*8 [constituent] !
```

The keyword is a compact way to simultaneously define a species, a *compound phase* (maximum 24 characters) and its phase-constituent. It is useful for stoichiometric phases with constant compositions. The species name and stoichiometric formula must be identical, i.e. being the given *constituent*. The phase has this species as its only constituent. This keyword allows the database definition file for a large substance database to be more compact; it is a combination of the *SPECIES* on page 8, *PHASE* on page 9 and *CONSTITUENT* on page 14 keywords.

### Examples

```
COMPOUND_PHASE AL2O3 % AL2O3 !
COMPOUND_PHASE MAGNETITE %MF FE3O4 !
COMPOUND_PHASE QUARTZ % SIO2 !
```

## ALLOTROPIC\_PHASE

```
ALLOTROPIC_PHASE [phase name]*24 [data-type code]*8 [constituent] !
```

This keyword does the same as the *COMPOUND\_PHASE* above keyword for entering an allotropic phase (maximum 24 characters), but does not enter the constituent as a species to the data structure. Use this if the species is already defined.

### Examples

```
ALLOTROPIC_PHASE BETHA-AL2O3 % AL2O3 !
ALLOTROPIC_PHASE CRISTOBALITE % SIO2 !
ALLOTROPIC_PHASE TRIDYMITE % SIO2 !
```

## TEMPERATURE\_LIMITS

```
TEMPERATURE_LIMITS [lower limit] [upper limit] !
```

This keyword sets the default upper and lower temperature limits used by the GIBBS module for Gibbs energy parameters and functions. It can be used only once in one database definition file and all its sequential files.

### Example

```
TEMPERATURE_LIMITS 500.0 1800.0 !
```

## DEFINE\_SYSTEM\_DEFAULT

```
DEFINE_SYSTEM_DEFAULT [keyword] {G-ref. type index} !
```

This keyword sets the default value to ELEMENT or SPECIES in the DATA command [DEFINE\\_SYSTEM](#) on [page 15](#) in the *Thermo-Calc Console Mode Command Reference*.

For a substance database, it can be appropriate to have ELEMENT as a default value whereas a large solution database can benefit from having SPECIES as a default value. A proper default value is useful for beginners. An advanced user is more likely to use the DATA commands DEFINE\_ELEMENT and DEFINE\_SPECIES to override the default value.

{*G-ref. type index*} is an integer indicating the reference state type for an element when entering and listing data in the GIBBS module. The following lists legal numbers and the corresponding meaning (the reference state type for an element):

Number	Definition
1	symbol: G
2	symbol: H298
3	symbol: H0

### Example

```
DEFINE_SYSTEM_DEFAULT element 2 !
```

## DEFAULT\_COMMAND

```
DEFAULT_COMMAND [secondary keyword and parameters] !
```

This keyword specifies commands to be executed by the DATA module at database initialization. The syntax of the available command is currently not the same as the user available DATA commands but the actions are similar. The available *secondary keyword and parameters* in syntax are:

```
DEFINE_SYSTEM_ELEMENT [element names]
DEFINE_SYSTEM_SPECIES [species names]
DEFINE_SYSTEM_CONSTITUENT [phase] [sublattice] [species]
REJECT_SYSTEM_ELEMENT [element names]
REJECT_SYSTEM_SPECIES [species names]
REJECT_SYSTEM_CONSTITUENT [phase] [sublattice] [species]
REJECT_PHASE [phase names]
RESTORE_PHASE [phase names]
```

### Examples

```
DEFAULT_COMMAND DEFINE_SYSTEM_ELEMENT FE VA !
DEFAULT_COMMAND REJECT_SYSTEM_CONSTITUENT LIQUID 2 C !
```

```
DEFAULT_COMMAND REJECT_PHASE LIQUID !
```

```
DEFAULT_COMMAND RESTOR_PHASE GAS !
```

## DATABASE\_INFORMATION

```
DATABASE_INFORMATION [text]*10000 !
```

This keyword defines a text for the detailed description of the current database. The text can be listed with the DATA command DATABASE\_INFORMATION. An apostrophe (') can be used in the text to indicate a new line; and two apostrophes, (') can be used in the text to indicate a new line plus an empty line.



The continuous *text* length (each line with max 78 characters) is 10,000 characters.

### Example

```
DATABASE_INFORMATION This is the XXX-Alloy Solution Database '
                      in the A-B-C-D-..... System. '
                      Developed by TCS, released in May 2001. ''
                      ... more ... !
```

## TYPE\_DEFINITION

```
TYPE_DEFINITION [data-type code]*1 [secondary keyword with
parameters] !
```

This keyword couples phases to an action performed by the DATA module when the DATA command [GET\\_DATA](#) on page 15 is executed.

### Secondary Keywords

The secondary keywords and associated parameters in syntax are:

```
SEQ [filename]
RND# [filename]
GES [valid GIBBS command with parameters]
POLY3 [valid POLY command with parameters]
TDB [valid DATA command with parameters]
IF [conditional statement] THEN [keyword with parameters]
AFTER [valid GIBBS command with parameters]
```

The secondary keyword `SEQ` specifies a sequential file that stores parameters belonging to the phases using the associated data type code (which is defined by this keyword). A special case where the filename is given as an asterisk (\*) implies that the database definition file also acts as a sequential data storage file. This case makes it possible to have a single file for a small database, which is especially suited for personal databases.

The secondary keyword `RND` should be concatenated with a positive integer # to indicate the type of the random file. Currently, there are these types of random files:

- `RND0`, the default, is used for complete Gibbs energy expressions (G0 parameters), where the search field is the unabbreviated parameter name.
- `RND1` is designated for functions, where the function name is used as the search field.
- `RND2` is reserved for binary interaction parameters, where its search field is also the unabbreviated parameter name without any interaction order notation.



Ternary and higher order interaction parameters must be specified on a sequential file. Moreover, the internal structures of these random files are subject to changes with different versions of DATA, and with implementations of DATA on various computer systems. For more information, see the FORTRAN program TDBSORT, which is available from Thermo-Calc Software AB.

The secondary keywords `GES`, `POLY3`, or `TDB` specifies a modification of, or addition to, phases having the associated data type code, such as magnetic contribution, another excess model, or any other valid GIBBS/POLY/DATA command that applies to a certain phase. By implementing this as a call to the interactive GIBBS/POLY/DATA module, flexibility is achieved. If a new type of addition is implemented in a GIBBS/POLY/DATA module, it can be immediately used in the database definition file without reprogramming the DATA module.



In several examples below, the use of the at (@) sign indicates any phase to which the relevant type definition (e.g. A, B, 4, or E) applies.

The secondary keywords `IF` and `THEN` allow specification of a conditional statement structured with respect to the phase constitution that controls the execution of a following type-definition (keyword with parameters) string. See the last four examples.

The secondary keyword `AFTER` is similar to the `GES` keyword except the defined GIBBS command is executed after all parameters are entered. The reason for this is that the command has no effect unless there is a parameter. Following the `AFTER` keyword, a GIBBS command must be given and it is executed after entering the parameters of the phase.

The data-type code (always as one string) can be any normal or special character, e.g. 0, 5, A, F, M, %, &, and so forth, and is referred in the definition keywords [PHASE on page 9](#), [COMPOUND\\_PHASE on page 16](#) and [ALLOTROPIC\\_PHASE on page 16](#) for various phases.

A phase can have several ADDITIONAL parts of different types (that are enforced by certain TYPE\_DEFINITIONS which call the GIBBS command AMEND\_PHASE\_DESCRIPTION for describing various contributions to Gibbs energy). However, the DATA/GIBBS module automatically deletes any early-defined ADDITIONAL part(s) of the same type.

The DATA module can selectively retrieve functions that are necessary for a defined system from a database that has functions stored in its `setup` file or `SEQ` sequential function file, while all other functions irrelevant for the defined system are ignored and are not saved in associated GIBBS and POLY workspaces.

### Examples

```

TYPE_DEF % SEQ TCPATH\DATA\[DATABASE]\PARAMETERS.TDB !
TYPE_DEF I SEQ TCPATH\DATA\[DATABASE]\INTERACTION-PARAMS.TDB !
TYPE_DEF G RND0 TCPATH\DATA\[DATABASE]\GZERO-PARAMS.TDB !
TYPE_DEF F RND1 TCPATH\DATA\[DATABASE]\FUNCTIONS.TDB !
TYPE_DEF & RND2 TCPATH\DATA\[DATABASE]\BINARY-INTERACTIONS.TDB !
TYPE_DEF A GES AM_PH_DES @ MAGNETIC -1 0.40 !
TYPE_DEF B GES AM_PH_DES @ MAGNETIC -3 0.28 !
TYPE_DEF 4 GES AM_PH_DES @ EXCESS_MODEL REDLICH-KISTER_KOHLER !
TYPE_DEF 5 GES AM_PH_DES AQUEOUS EXCESS_MODEL HKF !
TYPE_DEF 6 GES AM_PH_DES AQUEOUS HKF_ELECTROSTATIC !
TYPE_DEF 7 GES AM_PH_DES AQUEOUS STATUS 02084000,,, !
TYPE_DEF 8 GES AM_PH_DES AQUEOUS MAJOR_CONST 1 H2O !
TYPE_DEF E AFTER AM_PH_DES LIQUID EXCESS MIXED-EXCESS
      A B LEGENDRE C A POLYNOM ,,,, !
TYPE_DEF T AFTER AM_PH_DES LIQUID TERN-EXT TOOP-KOHLER B A C ,,,, !
TYPE_DEF Q AFTER AM_PH_DES LIQUID TERN-EXT KOHLER FE CR NI !
TYPE_DEF C IF (PD AND PT AND SN) THEN TDB RESTORE_PHASE BCT_A5 !
TYPE_DEF D IF (PD AND (PT OR SN)) THEN TDB REJECT_PHASE BCC_A2 !
TYPE_DEF E IF ((NB OR TI OR V) AND (C OR N)) THEN
      GES AM_PH_DES @ COMP_SET ,, CR NB TI V: C N: !
TYPE_DEF F IF (ALO3/2 OR CRO3/2 OR FEO OR MNO OR SIO2) THEN
      GES AM_PH_DES LIQUID COMP_SET ,, ALN%,ALO3/2%,CRO3/2%,
      FEO%,FEO3/2%,MNO3/2%,MNS%,SIO2%,TIO2% : !
TYPE_DEF R GES AM_PH_DES FE_LIQUID FRACTION_LIMITS Fe 0 0.6
      Ag 0 0.01 Al 0 0.05 Ca 0 0.05 Co 0 0.01 Cr 0 0.01
      Cu 0 0.02 Mg 0 0.05 Mn 0 0.05 Mo 0 0.05 Nb 0 0.05
      Ni 0 0.05 Pb 0 0.05 Si 0 0.10 Sn 0 0.02 Ti 0 0.05
      U 0 0.01 V 0 0.02 W 0 0.02 Zr 0 0.03
      B 0 0.01 C 0 0.01 H 0 0.01 N 0 0.01 O 0 0.01

```

```
P 0 0.01 S 0 0.01 !
```

## Ordered Phase Restores Disorder Contribution

When an ordered phase with disordered contribution is restored, the disordered contribution is automatically restored as well. You can also restore the disordered phase *without* restoring the ordered phase.



However the DIS\_PART TYPE\_DEFINITION must always be set on the ordered phase. It is important that the disordered phase is declared *before* the ordered phase. Otherwise it causes an error when DIS\_PART TYPE\_DEFINITION is executed and then either the ordered or disordered phase is rejected.

## Example

```
TYPE_DEFINITION & GES A_P_D FCC_A1 MAGNETIC -3.0 2.80000E-01 !
PHASE FCC_A1 %& 2 1 1 !
    CONSTITUENT FCC_A1 :CR,NI% : C%,VA : !
$ THIS PHASE HAS A DISORDERED CONTRIBUTION FROM FCC_A1
TYPE_DEFINITION ' GES AMEND_PHASE_DESCRIPTION FCC_L12 DIS_PART FCC_
A1,,,!
TYPE_DEFINITION ( GES A_P_D FCC_L12 MAGNETIC -3.0 2.80000E-01 !
PHASE FCC_L12 %'( 3 .75 .25 1 !
    CONSTITUENT FCC_L12 :CR,NI% : CR,NI% : C,VA% : !
```

For example a GES command such as the following only affects phases defined above or at the phase with this TYPE\_DEFINITION in the TDB file:

```
TYPE_DEFINITION ( GES A_P_D FCC_L12 DIS_PART FCC_A1,,,! !
```

For example a TDB command such as the following only affects phases defined *below* the phase with this TYPE\_DEFINITION in the TDB file:

```
TYPE_DEFINITION ( TDB RESTORE_PHASE FCC_A1 !
```

## FTP\_FILE

```
FTP_FILE [filename] !
```

FTP\_FILE is a special function random file and the function names correspond to the record numbers where these record names and the functions are stored. The FTP\_FILE decreases search time for the associated database in the DATA module. The file is used for large substance databases along with a SEQ sequential or RND0 random file for storage of G0 parameters referring the functions named FxxxxT that are stored in the FTP file. The integer number xxxx is a search code used by DATA when such files are processed.





No modification of this file type is allowed.

### Example

```
FTP_FILE TCPATH\DATA\[DATABASE]\FTP-FILE.DATA !
```

## FUNCTION

```
FUNCTION [function name]*8 [lowest temp. limit]
[expression 2]; [upper temp. limit 2] Y
[expression 1]; [upper temp. limit 1] Y
[expression 3]; [upper temp. limit 2] Y
..... ; ..... Y
[expression n-1]; [upper temp. limit n-1] Y
[expression n]; [upper temp. limit n] N {Ref. Index} !
```

GIBBS can use predefined functions in the expression (TP-Function) of a Gibbs energy parameter or in other functions. This is often used when several parameters (or functions) have a common sub-expression, such as for metastable modifications of elements. This keyword can appear in both files for database definition and sequential storage, but not in FTP files. A valid *function name* can have up to 8 characters.

A function always starts with a lowest temperature limit of its applicability, followed by one or more (up to 10) expressions (TP-Functions) that are coded as mathematical relations of constants, functions of stable variables (T and P) and other entered functions (normally with a # suffix, e.g. +3\*GHSERAL#).



Also see the [ENTER\\_PARAMETER](#) on page 99 in the *Thermo-Calc Console Mode Command Reference*.

The expression is a FORTRAN-like expression and operators +, -, \*, = and \*\* can be used (\*\* only with integer powers). Unary-functions LN or LOG (both for natural logarithm) and EXP (for exponential) can also be used. Each expression (TP-Function) should end with a semicolon (;), and be followed by its upper applicable temperature limit and a continuation indicator (Y to continue with the next expression or N to end the function's expression). If there is no continuation after a specific expression (TP-Function), the reference index can optionally be given after the N indicator.

A complete/valid function entry can be written in several continuation lines if the function's expression (TP-Function) is too long or if there is more than one applicable expression (TP-Function), as the maximum length of each line is 78 characters.



It is recommended to always have at least one empty space at the beginning of each continuation line. Otherwise, the DATA module may misunderstand the expression or issue some error messages when reading the function entry. Avoid entering functions like the one below.

```
FUNCTION GHSERXY 298.15
-1000+1058*T-38.9*T*LOG(T)+GFUNXY#; 6000 N !
```

Such a function is read by the DATA module as

```
1000+1058*T-38.9*T*LOG(T)+GFUNXY#
```

rather than

```
-1000+1058*T-38.9*T*LOG(T)+GFUNXY#
```

This is because the DATA module concatenates all lines and removes extra spaces before trying to enter the function in the GIBBS workspace. Thus, the – sign is taken as a delimiter between 298.15 and 1000, and the function incorrectly becomes:

```
FUNCTION GHSERXY 298.15 1000+1058*T-38.9*T*LOG(T)+GFUNXY#; 6000 N !
```

Avoid this mistake by giving at least one empty space as the first character of a new line, such as

```
FUNCTION GHSERXY 298.15
-1000+1058*T-38.9*T*LOG(T)+GFUNXY#; 6000 N !
```

which is read correctly as

```
FUNCTION GHSERXY 298.15 -1000+1058*T-38.9*T*LOG(T)+GFUNXY#; 6000 N !
```

The lowest-temperature limit (in Kelvin) for the applicability of the (first) TP-Function in a function is normally set by default as 298.15 K, in most cases. However, you can set another limit when it is applicable (according to experimental data and assessments).

An upper-temperature limit (in Kelvin; followed by a Y or N sign) for the applicability of each TP-Function in a function must be given after the semicolon (;) immediately following the specific TP-Function. The highest-temperature limit (in Kelvin) for the applicability of the current function is always followed by the N sign. If a negative number is given as the lowest-temperature limit, it assumes there are breakpoints in pressure for this function. In these cases, it is interpreted as the lowest-pressure limit (in Pascal), and the other limits in the current function is also taken as pressure limit values (in Pascal).

The temperature/pressure limits for the functions are checked during calculations. An indicator is set if the actual temperature/pressure condition is below the lowest temperature/pressure limit or above the highest temperature/pressure limit. In these cases, an extrapolation is done using the TP-Function valid in the nearest temperature/pressure range.

The optional reference index {*Ref. Index*} is an integer number indicating where to find the particular function in a special reference file. The references are listed when doing the GET\_DATA command in the

DATA module. They can also be listed in the GIBBS module with the command LIST\_DATA with the option R.



For accounting for the reference indices, also see the keyword [REFERENCE\\_FILE](#) on page 35.

The reference index field can also be an abbreviation (such as REF:250, REF\_002, or REF-SGTE) which denotes the original reference. In this case, the reference cannot be obtained when issuing the DATA command GET\_DATA or the GIBBS command LIST\_DATA (with the option R).

However, the references directly coded in the database definition file (`***setup.TDB`) starting with a letter can be shown when issuing the DATA command GET\_DATA or the GIBBS command LIST\_DATA (with the option N or R). Normally, such references must be located after the LIST\_OF\_REFERENCE keyword. It is recommended to use reference code names such as REF001, REF018, etc. The reference list, which is generated by the GIBBS command [LIST\\_DATA](#) on page 77 <file> with the N or R option, is also possible to be directly read by the DATA module.

The DATA module can selectively retrieve functions which are necessary for a defined system from a database that has functions stored in its setup file or SEQ sequential function file, while all other functions irrelevant for the defined system are ignored and are not saved in associated GIBBS and POLY workspaces. Previously, this can only be done for large databases that have functions stored in RND1 random or FTP function files.

## Examples

```
FUNCTION GFREE 298.15 1000+GFUNXY#; 6000 N !
FUNCTION GFUNXY 298.15 -1000+200*T+30*T*LOG(T); 6000 N 505 !
FUNCTION GO_CAO 298.15 -663538.11+352.67749*T-57.7533*T*LN(T)
+5.3895E-03*T**2-8.879385E-07*T**3+575530*T**(-1);
1400.00 Y -625196.99+78.896993*T-20.40145*T*LN(T)
-1.112923E-02*T**2+5.1896733E-07*T**3-6917350*T**(-1);
2900.00 Y -499226.55-490.37695*T+51.95912*T*LN(T)
-2.961051E-02*T**2+1.4033905E-06*T**3-48114685*T**(-1);
3172.00 Y -587711.89+375.04117-62.76*T*LN(T);
6000.00 N REF020 !
```

## PARAMETER

```
PARAMETER [GIBBS parameter name] [lowest temp. limit]
[expression 1]; [upper temp. limit 1] Y
[expression 2]; [upper temp. limit 2] Y
[expression 3]; [upper temp. limit 2] Y
..... ; ..... Y
```

---

```
[expression n-1]; [upper temp. limit n-1] Y
[expression n]; [upper temp. limit n] N {Ref. Index} !
```

This keyword can appear in both files for database definition and sequential storage, but not in FTP files. After the keyword, a valid *GIBBS parameter name* should be given.

It is used to define standard Gibbs energies (i.e. the **G** parameters for Gibbs energy of formations) of all valid end-members of various stoichiometric and solution phases, and excess Gibbs energies (i.e. the **L** parameters for Gibbs energy of interactions) of all binary, ternary, quaternary or higher-order interactions in various solution phases; both standard Gibbs energies and excess energies can also have parameters for contributions from PT-depended volume variations (i.e. the **V0**, **VA**, **VB**, **VC** and **VK** parameters for molar volume, thermal expansivity, bulk modulus, isothermal compressibility and high-pressure fitting parameter), magnetic ordering (i.e. the **TC** and **BM** parameters for Curie temperature and Bohr magneton number) and hypothetical electrostatic interactions (i.e. **BM** parameter for Born functions  $\omega_{Pr,Tr}$  of aqueous solute species).

The general form of a parameter is:

```
<identifier>(<phase>, <constituent array>; <digit>) <xxx>
<expression> <yyy> <keyword Y or N> <zzz> !
```

## General Form

Name	Description
identifier	The parameter type.
phase	The phase name (maximum 24 characters).
constituent array	The specific constituent array in the phase.
digit	The degree of composition-dependent interaction contribution (an integer number from 0 through 9), that is only for excess energy (L), Curie temperature (TC) and Bohr magneton number (BMAGN), as well as for volume-related parameters (V0 or VA or VB or VC or VK); if it is valued as zero, or if it is for the standard Gibbs energy (G) for which the degree is always zero, it can be omitted.
expression	The mathematical relation to describe the parameter.
xxx and yyy	The low and high temperature limits respectively for the applicable temperature range of the parameter expression
keyword Y or N	The indicator on if there is continuation for the parameter expression or not
zzz	The reference index/number for the assessment of this parameter;
!	The exclamation mark is used to indicate that the current parameter definition is ended

## GIBBS Parameter Name

The GIBBS parameter name has a general form of:

`<identifier>(<phase>,<constituent array>;<digit>)`

## Name Examples

Parameter	Definition
G (GAS, C1O2)	The Gibbs energy of formation of a CO2 molecule in gas.
G (FCC, Fe:VA)	The Gibbs energy of formation of fcc Fe with interstitials.
L (LIQ, Fe,Cr;0)	The regular solution parameter for Fe and Cr in liquid.
L (LIQ, Fe,Cr;1)	The sub-regular solution parameter.
TC (BCC, Fe:Va)	The Curie temperature of bcc Fe.
BMAGN (BCC, Fe:Va)	The Bohr magneton number parameter of bcc Fe.

The GIBBS parameter name consists of several parts. The first is a *type-identifier*. The following type-identifiers are legal:

Type-Identifier	Definition
G	Standard energy parameter (Gibbs energy of formation)
L	Excess energy parameter (Gibbs energy of interaction)
TC	Curie temperature for magnetic ordering
BMAGN or BM	Bohr magneton number for magnetic ordering (or Born function $\omega_{Pr,Tr}$ for aqueous solute species).
V0	Molar volume at 298.15 K and 1 bar (a numeric value only)
VA	Integrated thermal expansivity $\int_{298.15}^T \alpha(T) dT$
VB	Bulk modulus at 1 bar
VC	Isothermal compressibility
VK	High-pressure fitting parameter

You can also use G for interaction parameters; and on output list (performed by the GIBBS command LIST\_PARAMETER or LIST\_PHASE\_DATA) the type-identifier L is always used for interaction parameters. Note that the type-identifier BM is also used for Born functions  $\omega_{Pr,Tr}$  of aqueous solute species.

The identifier must be followed by an opening parenthesis, a phase name, a comma and a constituent array. Optionally, the constituent array can be followed by a semicolon and a digit. The parameter name is terminated by a closing parenthesis.



It is important that if a phase bears a legal phase-type (among G, A, Y, L, I, F and B) in its phase definition (already by the PHASE keyword; such as GAS:G, LIQUID:L, SLAG:L, IONIC\_LIQ:Y, SPINEL:I, FCC\_L12:F, HCP\_D021:F, BCC\_B2:B, AQUEOUS:A), such a valid phase-type code should not be attached to the phase name in the PARAMETER keyword.



Specifying the phase name in UPPER-case is recommended. You can define a phase name as a mixture of UPPER-case and lower-case letters in a database, but the DATA module automatically converts all lower-case to UPPER-case because the GIBBS module only recognizes UPPER-case phase names.

The *constituent array* consists of a list of constituent names. Interaction parameters have two or more constituents from the same sublattice separated by a comma. If the phase has sublattices, at least one constituent in each sublattice must be specified. The constituents in different sublattices must be given in sublattice order and are separated by a colon.

After the component array, a sub-index digit can be specified after a semicolon. This digit must be in the range 0 to 9. The interpretation of the sub-index depends on the excess energy model used for the phase. If no semicolon and digit are given, the sub-index value is assumed to be as zero.

The excess energy parameters, e.g. the regular/subregular (binary) parameter or ternary parameters, are multiplied with two or more fractions of the constituents from the same sublattice of the solution phase. These additional constituents must be given as interacting constituents.



Be careful about the sign of odd terms, for example,  $L(\text{BCC}, \text{B}, \text{A:VA}; 1)$  is treated as  $L(\text{BCC}, \text{A}, \text{B:VA}; 1)$ , i.e. it is always put into alphabetical order.



Solution phases with sublattices may have interacting constituents in each sublattice.

You can use an asterisk (\*) to denote that the excess interaction parameter is independent of the constituents of a specific sublattice. For example,  $L(\text{FCC\_L12}, \text{AL}, \text{NI}; *)$  means that the interaction parameter is for the binary interaction between constituents AL and NI on the first sublattice in the FCC\_L12 solution phase, while it is independent of all constituents on the second sublattice. A interaction parameter in the list of constituents is always added to the Gibbs energy and the asterisk (\*) is calculated with the term of  $[1 - \sum y(\text{specified constituents})]$ , which implies that in an A-B binary system the following three  $L$  parameters are identical (but in higher-order systems, they are different):

- $L(\text{phase}, \text{A}, \text{B})$  is multiplied with  $X(\text{A}) * X(\text{B})$
- $L(\text{phase}, \text{A}, *)$  is multiplied with  $X(\text{A}) * (1 - X(\text{A}))$
- $L(\text{phase}, \text{B}, *)$  is multiplied with  $X(\text{B}) * (1 - X(\text{B}))$

A parameter always starts with a lowest temperature limit of its applicability, followed by one or more (up to 10) expressions (TP-Functions) coded as mathematical relations of constants, functions of stable variables (T and P) and entered functions (normally with a # suffix, e.g.  $+3 * \text{GSERAL}\#$ ).

The expression is a FORTRAN-like expression and operators +, -, \*, = and \*\* can be used (\*\* only with integer powers). Unary-functions LN or LOG (both for natural logarithm) and EXP (for exponential) can also be used. Each expression (TP-Function) should ends with a semicolon (;) and be followed by its upper applicable temperature limit and a continuation indicator (Y to continue with the next expression, or N to end the parameter's expression). If there is no continuation after a specific expression (TP-Function), the reference index can be optionally given after the N indicator.

A complete/valid parameter entry can be written in several continuation lines if the parameter's expression (TP-Function) is too long or if there is more than one applicable expression (TP-Function), as the maximum length of each line is 78 characters.



It is recommended to always have at least one empty space at the beginning of each continuation line. Avoid entering parameters such as:

```
PARAMETR G(LIQUID,A,B) 298.15
-2000+4568*T+2*GFUNAB#; 6000 N !
```

Such a parameter is read by the DATA module as 2000+4568\*T+2\*GFUNAB#, rather than as -2000+4568\*T+2\*GFUNAB#.

Avoid this mistake by giving at least one empty space as the first character of a new line, such as

```
PARAMETR G(LIQUID,A,B) 298.15
 -2000+4568*T+2*GFUNAB#; 6000 N !
```

The lowest-temperature limit (in Kelvin) for the applicability of the (first) TP-Function in a parameter is normally set by default as 298.15 K, in most cases; however, you can set another limit when it is applicable (according to experimental data and assessments). An upper-temperature limit (in Kelvin; followed by a **Y** or **N** sign) for the applicability of each TP-Function in a parameter must be given after the semicolon (;) immediately following the specific TP-Function; and the highest-temperature limit (in Kelvin) for the applicability of the current parameter is always followed by the **N** sign. If a negative number is given as the lowest-temperature limit, it is assumed that there are breakpoints in pressure for this parameter. In such cases, it is interpreted as the lowest-pressure limit (in Pascal), and the other limits in the current parameter are also taken as pressure limit values (in Pascal).

The temperature/pressure limits for the parameters are checked during calculations. An indicator is set if the actual temperature/pressure condition is below the lowest temperature/pressure limit or above the highest temperature/pressure limit. In these cases, an extrapolation is done using the TP-Function valid in the nearest temperature/pressure range.

The optional reference index {*Ref. Index*} is an integer number indicating where to find the particular parameter in a special reference file. The references are listed when doing the GET\_DATA command in the DATA module. These can also be listed in the GIBBS module with the command LIST\_DATA and the option **R** or **N**.



For accounting the reference indices, also see the keyword [REFERENCE\\_FILE](#) on page 35.

The reference index field can also be an abbreviation (such as REF:250, REF\_002, or REF-SGTE) denoting the original reference. In this case, the reference cannot be obtained when issuing the DATA command GET\_DATA or the GIBBS command LIST\_DATA (with the option **R** or **N**).



However, the references directly coded in the database definition file (`***setup.TDB`) that starts with a letter can be shown when issuing the DATA command `GET_DATA` or the GIBBS command `LIST_DATA` (with the option `R` or `N`). Normally, such references must be located after the `LIST_OF_REFERENCE` keyword. It is recommended to use reference code names such as `REF001`, `REF018`, etc. The reference list, which is generated by the GIBBS command `LIST_DATA <file>` with the `N` option, is thus also possible to be directly read by the DATA module.

## Examples

```

PARAMETER G (BCC,FE:VA) 298.15 1000+200*T+...; 6000 N 91DIN !
PARAMETER TC (BCC,FE:VA) 298.15 +1043; 6000 N 91DIN !
PARAMETER BMAGN (BCC,FE:VA) 298.15 +2.22; 6000 N 91DIN !
PARAMETER G (SIGMA,FE:CR:CR;0) 298.15 1000+200*T+...; 6000 N 101 !
PARAMETER G (LIQUID,AL;0) 298.15 +11005.553-11.840873*T
+7.9401E-20*T**7+GHSERAL#;
933.60 Y +10481.974-11.252014*T+1.234264E+28*T**(-9)+GHSERAL#;
2900.00 N REF:283 !
PARAMETER G (BCC_A2,PB:C) 298.15 UN_ASS#; 300 N REF:0 !
PARAMETER G (BCC_A2,NI:C;0) 298.15 +GHSERNI#+3*GHSERCC#
+400000-100*T; 6000 N REF071 !
PARAMETER G (BCC_A2,MN:VA) 298.15 +GMNBCC#; 6000 N REF285 !
PARAMETER BM (AQUEOUS,OH-1) 298.15 +Z0002PW0#; 1600 N 155 !
PARAMETER L (BCC,FE,CO:VA;0) 298.15 1000+200*T+...; 6000 N !
PARAMETER L (BCC,FE,CO:VA;1) 298.15 1000+200*T+...; 6000 N !
PARAMETER L (BCC,FE,CO:VA;2) 298.15 1000+200*T+...; 6000 N !
PARAM TC (BCC_A2,CO,MO:VA;0) 298.15 -3700; 6000 N R454 !
PARAM TC (BCC_A2,CO,MO:VA;1) 298.15 +2300; 6000 N R454 !
PARAM BMAGN (BCC_A2,CO,MO:VA;0) 298.15 -3.445; 6000 N R454 !
PARAM V0 (BCC_A2,CR,FE:VA;0) 298.15 +ZERO#; 6000 N REF06V !
PARAM V0 (BCC_A2,CR,FE:VA;1) 298.15 -1.10524097E-7; 6000 N REF06V !
PARAM V0 (BCC_A2,CR,FE:VA;2) 298.15 +1.40024130E-7; 6000 N REF06V !
PARAM VA (BCC_A2,CR,FE:VA;0) 298.15 -6.49444634E-6*DELTAT#; 6000 N
REF06V !
PARAM VA (BCC_A2,CR,FE:VA;1) 298.15 +2.91269321E-5*DELTAT#; 6000 N
REF06V !

```

## OPTIONS

```

OPTIONS /[alloy name]([composition limitations for all alloying
elements]) !

```

This keyword defines an alloy in a database. An alloy has a name, a major component and a number of alloying elements. The purpose for defining an alloy is to be able to tell you about applicable composition limits of the current database in applications to that particular type of alloy. It is possible to have several alloys in the same database. The alloys are given after the keyword in the database.

The alloy name must be preceded by a slash (/) and terminated by the opening parenthesis, with no spaces are allowed in between.

- The alloy name is maximum 8 characters.
- After the parenthesis, follows the major element and a parenthesis with its minimum mass and minimum mole percent given inside.
- Then, the alloying element names, each with its maximum mass and mole percent are given within parenthesis.
- There must a space between definitions for each alloying element.
- The alloy definition is terminated by a closing parenthesis, and the whole OPTIONS keyword by the exclamation mark (!).

### Example

```
OPTIONS /SSteel(Fe(60,60) CR(30,30) NI(15,15) SI(1,1) N(.1,1)) !
```

## TABLE



It is recommended to always have at least one empty space at the beginning of each continuation line. Otherwise, the DATA module may issue some error messages when reading the table entry.

```
TABLE [name]*8 [start temp] [end temp] [delta temp] [table values] !
```

This keyword can appear in both files for database definition and sequential storage, but not in FTP files. It makes a table of Gibbs energy as a function of temperature where the values are given from the start temperature to the end temperature, at a step of the delta temperature.

### Example

```
TABLE DENTAB 1000.0 1500.0 100.0 -2912.9008 -2834.2416 -2755.5824
-2677.7600 -2600.7744 -2524.2072 !
```

## ASSESSED\_SYSTEMS

```
ASSESSED_SYSTEM [descriptions on special treatments for specific
assessed systems]*8000 !
```

This keyword can be included in the database definition file (the `***setup.TDB` file). A maximum of 8000 characters after the keyword (to describe some special options when the DATA, GIBBS and POLY models deal with the existing systems with assessed data) is allowed until the exclamation mark (!).

Several ASSESSED\_SYSTEMS keywords can be used in the same TDB file in order to have more lists of assessed systems. There is no limit to the number of the entries in the same TDB file.

The assessed systems in the database, and the special treatment options, are typed after the keyword. The elements (always in UPPER CASE) in each assessed system must be in alphabetical order and be separated by a hyphen, such as C-**FE** for the Fe-C binary system, and C-CR-**FE** for the Fe-Cr-C ternary system. A space must be between each assessed system. Information on assessed binary, ternary or higher-order systems may also be given in this way.



A ternary system like C-CR-**FE** does not imply that the binary C-CR, C-**FE** and CR-**FE** are assessed. There is no way to indicate partially assessed systems.

- There is a field to give some descriptive information for a specific system, with various options about how to:
  - Reject or restore phase(s) from the current database in the DATA module;
  - Set major constituent(s) in the first composition set and to set a second composition set for a specific phase available in the current database in the GIBBS module; *and*
  - Calculate this specific system in the POLY module.
  - This is the facility used by the BIN (binary phase diagrams) and TERN (ternary phase diagrams) modules in the Thermo-Calc software/database package.

The descriptive information must immediately follow the specific system name, and must be enclosed within parenthesis ( and ), and the left parenthesis must follow directly after the system, such as :

```
AL-NI (TDB +L12 ;G5 C-S:L12/NI:AL:VA ;P3 STP:.8/1200/1 STP:.2/600/1)
```

The syntax TDB means that the commands to the DATA module proceed, and +L12 in the example means that the phase called L12 should be restored (it has been rejected by default).

The directive ;G5 means that the following are commands to the GIBBS module. C\_S: means creating a second composition set, after the colon follows the phase name and after the slash the major constituents.

After the directive ;P3 follows commands to the POLY module. STP: means setting a start point with the value of the X-axis first (composition for the second element in a binary system), the slash separates the Y-axis value (temperature), and possibly one or more directions (-1, 1, -2 or 2).

A summary of the allowed syntax is:

TDB accepts

- +phase and -phase for restore/reject.
- ;G5 accepts
- MAJ:phase/constituent-array for major constituents of the first composition set.
- C\_S:phase/constituent-array for a second composition set.

- ;P3 accepts
- TMM:lt/ht for the low-/high-temperature limits (lt and ht; for instance TMM:500/4000) suitable for calculating phase diagrams and property diagrams of a binary system.
- \* for a default start point which is set as:
  - for a binary system: at the composition  $X(2^{\text{nd}} \text{ element}) = .1234$ , temperature  $T = 1100 \text{ K}$  and with the default directions; or
  - for a ternary system: at the compositions  $X(2^{\text{nd}} \text{ element}) = .1234$  and  $X(3^{\text{rd}} \text{ element}) = .1234$  and with the default directions.
- STP:x/t/d1/d2/d3 for a specific start point in a binary system which is set as at the composition  $X(2^{\text{nd}} \text{ element}) = x$  and temperature  $T = t$  (in K), and with the directions d1, d2 and/or d3.
- STP:x1/x2/d1/d2/d3 for a specific start point in a ternary system which is set as at the compositions  $X(2^{\text{nd}} \text{ element}) = x1$  and  $X(3^{\text{rd}} \text{ element}) = x2$  and with the directions d1, d2 and/or d3.
- The direction(s) can be defined as -1, 1, -2 or 2. If no direction is specified, all default directions are used (meaning no ADD command is enforced in the POLY module).
- If only one start point is specified, the direction(s) may be omitted; if more than one start points are specified, at least one direction for each start point must be given for all start points.

Each entry for a specific binary or ternary sub-system can be written in one or several lines (each line with 78 characters).

### Other Examples

```

ASSESSED_SYSTEMS

AL-NI (TDB +L12 +BCC_B2 ;G5 C_S:L12/NI:AL:VA
      ;P3 STP:.8/1000/1 STP:.45/700/1 STP:.7/700/1)

AL-PB (TDB -HCP -BCC
      ;G5 MAJ:LIQ/AL MAJ:FCC/AL:VA C-S:LIQ/PB C-S:FCC/PB:VA ;P3 *)

CR-FE (;G5 C-S:BCC/CR:VA ;P3 STP:.6/1200/1/-2/2)

AG-CU (;G5 MAJ:FCC/AG:VA C_S:FCC/CU:VA ;P3 STP:.3/1000)

C-NB (;P3 STP:.9/1100/1)

C-SI (;P3 *)

CO-CR (;G5 MAJ:FCC/CO:VA C_S:FCC/CR:VA ;P3 STP:.1/1100)

CR-FE (TDB -HCP ;G5 C_S:BCC/CR:VA ;P3 STP:.6/1200/1/-2/2)

```

```

CR-NI (;P3 *)
CR-W (;G5 MAJ:BCC/W:VA C_S:BCC/CR:VA
      ;P3 TMM:500/4000 STP:.3/700/1 STP:.3/1800/2 )
CU-FE (TDB -HCP ;G5 MAJ:LIQ/CU MAJ:FCC/FE:VA C_S:FCC/CU:VA
      ;P3 STP:.9/1400)
FE-N (TDB +FE4N ;P3 *)
FE-O (TDB -LIQUID +IONIC ;G5 C_S:ION_LIQ/FE+2:O-2 MAJ:ION_LIQ/FE+2:VA
      ;P3 STP:.2/2000/1 )
FE-S (TDB -LIQUID +IONIC ;G5 C_S:ION_LIQ/FE+2:S MAJ:ION_LIQ/FE+2:S-2
      ;P3 *)
AL-MG-SI (;P3 *)
C-CR-FE ;G5 MAJ:BCC/FE:VA C_S:BCC/CR:VA ;P3 *) !

```



The semicolon (;) is a part of the ;G5 and ;P3 directives. A long descriptive information can be written in more than one line, such as for the AL-NI, AL-PB, CU-FE and FE-O systems shown above.

The directive ;P3 \* is needed if the default start point should be used. If there is no P3 directive, the BIN or TERN module generates some 20 different start points in order to cover all possible compositions and temperatures (for a binary system) or all possible compositions (for a ternary system under any specific temperature).

## REFERENCE\_FILE

```
REFERENCE_FILE [file name] !
```

This keyword takes a reference file name as its argument. This reference file (that must be edited in a restrictive way and be saved as a blocked file with a fixed line-length for each line in the file, as described below) contains a complete list of the references for the various parameters (and sometimes functions) in the database. The file must have a fixed record structure: each reference entry with one or several records, and each record with exactly 78 characters written in one single blocked line; and no empty space is allowed at the beginning of all lines in the file. If there are more than one record entered for a reference entry, all the continuation lines must start with an ampersand (&). The line number of the first record for a specific reference entry is then accounted as the unique integer for that specific reference, which is referred when a parameter or function calls this integer as the optional {Ref. Index}.



Also see keyword [PARAMETER](#) on page 24 or [FUNCTION](#) on page 22 about specifying a reference index.

### Example

```
/-1<G>          T.C.R.A.S. Class 1
```

```

AG1.64TE1          THERMODATA 01/93
&28/01/93
&SILVER 1.64-TELLURIDE. Solid Standard State.
AG1                HULTGREN SELECTED VAL.          SGTE **
&AT.WEIGHT 107.870,STANDARD STATE:CODATA KEY VALUE.MPT=1234.93K. &--
U.D. 30/10/85.
AG1<G>             T.C.R.A.S   Class: 1
AG1/+1<G>          T.C.R.A.S   Class: 1
AG1BR1             N.P.L.                SGTE **
&Tfusion uncertain and heat vaporization estimated.
AG1BR1<G>          THERMODATA 01/93
&28/01/93
&Gaseous Standard State.
AG1BR103           BARIN & KNACKE.SUPPL.REF:62,* SGTE **
&AGO3BR   SILVER OXYTRIBROMIDE

```

In the example, the unique integers of related references (for assessed elements, species, phases, interactions, etc.) are:

```

1/-1<G>
2AG1.64TE1
5 AG1
8AG1<G>
9AG1/+1<G>
10AG1BR1
12AG1BR1<G>
15AG1BR103

```

## LIST\_OF\_REFERENCE

```

LIST_OF_REFERENCE
NUMBER SOURCE
    [REFxxx] '[Detailed reference]'
.....
..... !

```

This keyword starts a reference list that is directly coded in the database definition file (`***setup.TDB`). Its argument begins on the following line, and normally has an explanation line (NUMBER SOURCE) that is

followed by various reference codes. Each reference code may occupy one or more lines (each line with maximum 78 characters), but must have a reference code name (that starts with a letter) and the detailed reference information (that is written within two single-quotation marks, ' '). It is recommended to use reference code names such as REF001, REF018, etc. A maximum of 400,000 characters after the keyword is allowed until the exclamation mark (!).

Such a reference list can be shown when issuing the DATA command [GET\\_DATA on page 15](#) or the GIBBS command [LIST\\_DATA on page 77](#) (with the R option). The reference list, which is generated by the GIBBS command LIST\_DATA <file> with the N option, has this structure, and is thus possible to be directly read by the DATA module.

### Example

```
LIST_OF_REFERENCES
NUMBER  SOURCE
REF283  'Alan Dinsdale, SGTE Data for Pure Elements,
        Calphad Vol 15 (1991) p 317-425,
        also in NPL Report DMA(A)195 Rev. August 1990'
REF224  'P-Y Chevalier, Thermochimica Acta, 130 (1988) p 33-41; AG-SI'
!
```

### ADD\_REFERENCE

```
ADD_REFERENCE
[REFxxx] '[Detailed reference]'
.....
..... !
```

Use this keyword to have an unlimited number of references. The use of this is the same as that of [LIST\\_OF\\_REFERENCE on the previous page](#), and is used after it. Several ADD\_REFERENCES sections can be used in a single database if there are too many references.

It is recommended to always start with a so-called *empty reference* (such as the DUMP0 reference in the following example) as the first entry in each of the ADD\_REFERENCE sections to make sure that all references are listed appropriately as retrieving data by issuing the [GET\\_DATA on page 15](#) command.

### Example

```
ADD_REFERENCE
DUMP0  'Empty reference 0'
REF4   'J-O Andersson, B. Sundman, CALPHAD Vol 11, (1987), p 83-92
        TRITA 0270 (1986); CR-FE'
REF5   'J-O Andersson, Met. Trans A, Vol 19A, (1988) p 627-636
        TRITA 0207 (1986); C-CR-FE'
```



```

REFS 'Pingfang Shi (2006), TCS PTERN Public Ternary Alloys
Database,

      v1.2; Modified L0(BCC,Fe,C) and L0(BCC,Cr,C) parameters
      at high temperatures.'

... ..

!

ADD_REFERENCE

DUMP1 'Empty reference 1'

REF275 'A. Fernandez Guillermet, Z. Metallkde. Vol 79(1988) p.524-
536,

      TRITA-MAC 362 (1988); C-CO-NI AND C-CO-FE-NI'

REF393 'K. Frisk, Metall. Trans. Vol 21A (1990) p 2477-2488,

      TRITA 0409 (1989); CR-FE-N'

REF1096 'P. Gustafson, Metall. Trans. 19A(1988) p 2547-2554,

      TRITA-MAC 348, (1987); C-CR-FE-W'

... ..

!

```

## CASE and ENDCASE

```

CASE [ELEMENT/SPECIE/PHASE] !

  IF (boolean algebra on element, species or phase names) THEN

    [GIBBS/POLY/DATA command] !

ENDCASE !

```

This keyword takes as its argument, a definition on which type of the following Boolean algebra operates. A simple Boolean algebra using AND and OR with a maximum of four levels of parentheses works. The CASE construction must end with the ENDCASE keyword. This makes it possible to have additional GIBBS or POLY commands executed depending on the user selection of elements, species or phases. The DATA commands that can be given as secondary keyword to [DEFAULT\\_COMMAND](#) on page 17 can also be executed.

### Example 1

```

CASE ELEMENT !

  IF ((CR OR TI OR V) AND N)

    THEN GES AM_PH_DES @ C_S ,, CR MO TI V:C N: !

ENDCASE !

```

### Example 2

```

CASE ELEMENT !

```

```
        IF(O) THEN TDB DEFINE_SYSTEM_ELEMENT /- !  
    ENDCASE !
```

### Example 3

```
    CASE ELEMENT !  
        IF(AL AND FE)  
            THEN TDB DEF_SYS_ELEMENT VA !  
    ENDCASE !
```

## VERSION\_DATA

```
VERSION_DATE [string]*78 !
```

The string is denoted as the version/revision date and database manager of the database. Nowadays, this directive is used mainly for the purpose of keeping the development and revision history mostly updated.

### Example

```
VERSION_DATE Last update and adjustment: Database Manager, 2015-09-25  
!
```

---

## Working with the Mobility Databases

In this section:

---

<i>About the Diffusion Module (DICTRA) and the Databases</i> .....	<a href="#">41</a>
<i>Extensions to Database Definition File Syntax</i> .....	<a href="#">42</a>
<i>PARAMETER</i> .....	<a href="#">42</a>
<i>DIFFUSION</i> .....	<a href="#">43</a>
<i>ZERO_VOLUME_SPECIES</i> .....	<a href="#">43</a>

## About the Diffusion Module (DICTRA) and the Databases

A Diffusion Module (DICTRA) installation shares directories with Thermo-Calc, including the \DATA\ (or /data/) area and the database initiation file (TC\_INITD.TDB or initd.tdb).

When you want to switch or add self-generated databases/data-sets or any new database, use the predefined database list in the database initiation file as part of the Thermo-Calc installation packages.



You can add comment lines in the database initiation file, which must start with a \$ sign. These lines are ignored by the DATA module. This is also applicable if the database manager or user wants to temporarily disable a database in the predefined database list. If there are too many databases in the \DATA\ area that the DATA module cannot handle properly, the \$ sign can be used to temporarily comment about the uncommon databases. However, this does not often happen.

If Thermo-Calc is used with a Windows platform, such additional database initiation files can be located at any directory of any driver, on either a local computer or connected server. The NEW\_DICTORY\_FILE command displays an **Open** window to access a database initiation file if the file name or its path is not given on the same line of the NEW\_DICTORY\_FILE command, or if it is incomplete or incorrect, so that the path (in the Look in box) and database initiation file name (in the File name box) can be appropriately selected. However, if Thermo-Calc is run on a Linux/UNIX platform, these files must be located in the current working directory (where Thermo-Calc is started).

In an additional database initiation file, the first database entry may need to have the same path definition structure as in the ordinary database initiation file. Copy the entry line(s) for common databases from the original file to a database initiation file. The entries of the additional databases follow. Similar to the standard databases predefined in the database initiation file, all databases should normally be located in subdirectories under the directory as defined by the TCPATH parameter (Windows) or the TC\_DATA parameter (Linux/UNIX), or under its subdirectory \DATA\ or /data/.

### Windows Database Initiation File Example

For a Windows platform, the following example is an additional database initiation file, called MYINITD1.TDB:

```
$
$ DATABASES TCC (Additional TCC Databases)
PURE5 TCPATH\DATA\PURE5\PURE5SETU.TDB  SGTE Pure Elements Database,
version 5 !
AD1   TCPATH\DATA\ADD1\AD1SETUP.TDB      TCS ADD1 Solution Database,
version 1 !
AD2   TCPATH\ADDDATA\ADD2\AD2SETUP.TDB    TCS ADD2 Solution Database !
$AD2o TCPATH\ADDDATA\ADD2old\AD2SETUP.TDB TCS ADD2 Database (old) !
AD3   TCPATH\DATA\NEWDATA\ADD3\AD3SETUP.TDB TCS ADD3 Solution
Database !
```

```

AD4    TCPATH\DATA\NEWDATA\MYPROJ1\ADD4\AD4SETUP.TDB
      MYPROJECT1 ADD4 Solution Database !

$

$ DATABASES DIC (Additional DICTRA Databases)

DCAD1  TCPATH\DICDATA\DCADD1\DCAD1SET.TDB
      TCS DCADD1 Mobility Database !

```

## Extensions to Database Definition File Syntax

Software packages for simulation of diffusional phase transformations, such as the Diffusion Module (DICTRA) and Precipitation Module (TC-PRISMA), need both thermodynamic data and kinetic data (i.e. diffusivities or mobilities). Naturally, the handling and storage of kinetic data also benefits from the use of some kind of database management. Thus, the TDB database definition file syntax has been extended to incorporate some new keywords needed for storing kinetic data - [PARAMETER on page 24](#), [DIFFUSION on the next page](#), and [ZERO\\_VOLUME\\_SPECIES on the next page](#).

### PARAMETER

```

PARAMETER [special GIBBS parameter name] [low temp. limit]
[expression 1]; [upper temp. limit 1] Y
[expression 2]; [upper temp. limit 2] Y
[expression 3]; [upper temp. limit 2] Y
..... ; ..... Y
[expression n-1]; [upper temp. limit n-1] Y
[expression n]; [upper temp. limit n] N {Ref. Index} !

```

This keyword allows you to enter all types of normal GIBBS parameters for thermodynamic data as well as five special extensions suitable for kinetic data used in the Diffusion Module (DICTRA).

Valid extensions to special GIBBS parameter names are:

- MQ: Activation enthalpy for mobility equation.
- MF: Pre-exponential factor for mobility equation.
- DQ: Activation enthalpy for diffusivity equation.
- DF: Pre-exponential factor for diffusivity equation.
- VS: Volume counted per mole of volume carrying species.

### Examples

```

PARAMETER MQ (BCC, FE:VA) 298.15 1000+200*T+...; 6000 N !
PARAMETER MF (BCC, CO:VA) 298.15 1000+200*T+...; 6000 N !
PARAMETER DQ (FCC, FE:VA) 298.15 1043+...; 6000 N 10 !

```

```
PARAMETER DF(FCC,CR:C ) 298.15 1000+200*T+...; 6000 N 10 !
```

```
PARAMETER VS(FCC) 298.15 1000+200*T+...; 6000 N 11 !
```

## DIFFUSION

```
DIFFUSION [model keyword] [phase name] [additional parameter(s)] !
```

This keyword specifies the type of diffusion model to use for a phase if the default model is not desired. The default model calculates the full diffusion matrix. A diffusivity is calculated from the different mobilities and the thermodynamic factors. The former ones are calculated as:

$$M = \exp(\sum MF/RT) \exp(\sum MQ/RT) / RT$$

where  $\sum$  stands for a weighted summation of the different MF's and MQ's plus possibly a Redlich-Kister term.

### Valid Model Keywords

Keyword	Description
NONE	No diffusion in this phase
DILUTE	Constitution list of dependent species in each sublattice must be given as an additional parameter. Only the diagonal terms in the diffusion matrix are calculated. $D = \exp(\sum DF/RT) \exp(\sum DQ/RT)$ .
SIMPLE	Constitution list of dependent species in each sublattice must be given as additional parameter. Only the diagonal terms in the diffusion matrix are calculated. $D = \sum DF + \sum DQ$ .
MAGNETIC	The so-called ALPHA and ALPHA2 parameters must be given as additional parameters. ALPHA is for the substitutional magnetic model and ALPHA2 for the interstitial one. By appending an & sign and a species name after the alpha keyword one can supply individual values for the different species. The full diffusion matrix is calculated.

### Examples

```
DIFFUSION NONE SIGMA !
```

```
DIFFUSION DILUTE CEMENTITE : FE : C : !
```

```
DIFFUSION MAGNETIC BCC_A2 ALPHA=0.3 ALPHA2&C=1.8 ALPHA2&N=0.6 !
```

## ZERO\_VOLUME\_SPECIES

```
ZERO_VOLUME_SPECIES [list of species] !
```

In the Diffusion Module (DICTRA), the assumption that the volume is carried by the substitutional elements only is applied. The interstitial elements are assumed to have zero molar volumes. This keyword uses a list of which species are to be considered as zero volume ones for an argument.

### Example

```
ZERO_VOLUME_SPECIES VA C N !
```

---

## Database Definition File Examples

In this section:

---

<i>Example 1: A Steel Database .....</i>	<i>45</i>
<i>Example 2: A Custom Database for the Sb-Sn Binary System .....</i>	<i>46</i>
<i>Example 3: A Public Database for the Fe-Cr-C Ternary System .....</i>	<i>49</i>

## Example 1: A Steel Database

```

TEMP-LIM 500.0 2000.0 !

$

$ELEMENT, NAME, REF.STATE, ATOMIC-MASS, H0, S0 !

ELEMENT VA VACUUM          0.0    0.0 0.0 !
ELEMENT C  GRAPHITE        12.011  0.0 0.0 !
ELEMENT V  BCC              50.9415 0.0 0.0 !
ELEMENT CR BCC-PARAMAGNETIC 51.996  0.0 0.0 !
ELEMENT FE FCC-PARAMAGNETIC 55.847  0.0 0.0 !
ELEMENT NI FCC-PARAMAGNETIC 58.69   0.0 0.0 !
ELEMENT MO BCC              95.94   0.0 0.0 !
ELEMENT W  BCC              183.85   0.0 0.0 !

$

$PHASE, NAME, TYPE, NR-OF-SUBL, SITES-IN-EACH-SUBL. !

PHASE BCC      B1M  2 1.0 3.0 !
PHASE FCC      F2M  2 1.0 1.0 !
PHASE HCP      0    2 2.0 1.0 !
PHASE LIQUID   3    2 1.0 1.0 !
PHASE CEMENTITE 4    2 3.0 1.0 !
PHASE M23C6    4    2 23.0 6.0 !
PHASE M7C3     4    2 7.0 3.0 !
PHASE M6C      4    4 2.0 2.0 2.0 1.0 !
PHASE SIGMA    0    3 10.0 4.0 16.0 !
PHASE MU-PHASE 0    3 7.0 2.0 4.0 !
PHASE R-PHASE  0    3 27.0 14.0 12.0 !
PHASE GRAPHITE 4    1 1.0 !

$

$CONSTITUENT, PHASE-NAME : CONSTITUENTS !

CONSTITUENT BCC :V CR FE NI MO W:VA C: !
CONSTITUENT FCC :V CR FE NI MO W:VA C: !
CONSTITUENT HCP :CR FE NI:VA C N: !
CONSTITUENT LIQUID :C V CR FE NI MO W VA:VA C: !
CONSTITUENT CEMENTITE :CR FE:C: !
CONSTITUENT M23C6 :CR FE:C: !
CONSTITUENT M7C3 :CR FE:C: !
CONSTITUENT M6C :FE:W:FE W:C: !

```



```

CONSTITUENT SIGMA :FE:V CR MO:FE V CR MO: !
CONSTITUENT MU-PHASE :FE:MO W:FE MO W: !
CONSTITUENT R-PHASE :FE:MO :FE MO: !
CONSTITUENT GRAPHITE :C: !

$

$TYPE_DEFINITIONS:
TYPE-DEFINITION 0 SEQ TCPATH\DATA\METDATA\TC-THEREST.TDB !
TYPE-DEFINITION 1 SEQ TCPATH\DATA\METDATA\TC-BCC.TDB !
TYPE-DEFINITION 2 SEQ TCPATH\DATA\METDATA\TC-FCC.TDB !
TYPE-DEFINITION 3 SEQ TCPATH\DATA\METDATA\TC-LIQUID.TDB !
TYPE-DEFINITION 4 SEQ TCPATH\DATA\METDATA\TC-CARBIDES.TDB !
TYPE-DEFINITION M SEQ TCPATH\DATA\METDATA\TC-CURIE-BOHR.TDB !
TYPE-DEFINITION B GES AM-PH BCC MAGNETIC -1 .4 !
TYPE-DEFINITION F GES AM-PH FCC MAGNETIC -3 .28 !

$

$DEFAULT_COMMANDS:
DEFAULT-COMMAND DEF_ELEMENT VA !
DEFAULT-COMMAND REJ_SYS-CONST LIQUID 1 VA !

$DATABASE_INFORMATION:
DATABASE-INFO The following binary and ternary systems are available: '
    FE-CR-NI by Hertzman'
    FE-MO      Fernandez'
    FE-CR-C    Andersson'
    FE-W-C     Gustafson'
    FE-W       Andersson & Gustafson' !

```

## Example 2: A Custom Database for the Sb-Sn Binary System

```

$
$ELEMENT, NAME, REF.STATE, ATOMIC-MASS, H0, S0 !
ELEM VA VACUUM          0.0   0.0 0.0 !
ELEM MG HCP (A3)        24.305 0.0 0.0 !
ELEM SB RHOMBOHEDRAL (A7) 121.75 0.0 0.0 !
ELEM SN BCT (A5)        118.69 0.0 0.0 !
ELEM /- ELECTRON-GAS     0      0   0 !

$
$SPECIES, NAME, STOICHIOMETRIC-FORMULA !
SPECIE MG1 MG1!

```

---

```

SPECIE MG2 MG2!
SPECIE MG2+ MG/+2!
SPECIE SB1 SB1!
SPECIE SB2 SB2!
SPECIE SB4 SB4!
SPECIE SB3- SB/-3!
SPECIE SB5- SB/-5!
SPECIE SN1 SN1!
SPECIE SN4- SN/-4!

$
$PHASE, NAME, TYPE, NR-OF-SUBL, SITES-IN-EACH-SUBL. !
PHASE BCT          Z 1 1.0!
PHASE HCP          Z 1 1.0!
PHASE RHOMBO       Z 1 1.0!
PHASE GAS:G        Z 1 1.0!
PHASE LIQUID:L     Z 1 1.0!
PHASE IONICLIQ:Y   Z 2 1 1!
PHASE SPLIQ:Y      Z 2 1 1!
PHASE BMG3SB2:I    Z 2 3 2!
PHASE AMG3SB2:I    Z 2 3 2!
PHASE MG2SN:I      Z 2 2 1!
PHASE SBSN         Z 2 1 1!
PHASE SB2SN3       Z 2 2 3!

$
$CONSTITUENT, PHASE-NAME : CONSTITUENTS !
CONSTITUENT RHOMBO :SB SN:!
CONSTITUENT HCP :MG SN:!
CONSTITUENT BCT :SB SN:!
CONSTITUENT GAS:G :MG1 MG2 SB1 SB2 SB4 SN1:
    > Gas phase, using the Ideal EOS and Mixing Model. !
CONSTITUENT LIQUID:L :SB SN:!
CONSTITUENT IONICLIQ:Y :MG2+:SB SB3- SN SN4- VA:
    > This is the Ionic Liquid Solution Phase. !
CONSTITUENT SPLIQ:Y :MG2+:SB SB3- SN SN4- VA:!
CONSTITUENT BMG3SB2:I :MG2+:SB3- SB5- VA SN4-:!!
CONSTITUENT AMG3SB2:I :MG2+:SB3- VA SN4-:!!

```

---

---

```

CONSTITUENT MG2SN:I :MG2+ VA:SB3- SN4-:!  

CONSTITUENT SBSN :SB SN:SB SN:!  

CONSTITUENT SB2SN3 :SB:SN:!  

$  

$DEFAULT_COMMANDS:  

DEFAULT-COM DEF-ELEM VA /-!  

DEFAULT-COM REJ-PHASE LIQUID!  

DEFAULT-COM REJ-PHASE SPLIQ!  

$  

$TYPE_DEFINITIONS:  

TYPE-DEFINITION Z SEQ * !  

$  

$DATABASE_INFORMATION:  

DATABASE_INFO The Sb-Sn system with isentropic temperatures!  

$  

$VERSION_DATE:  

VERSION_DATE Last update 1986-05-18 11:39:49 !  

$  

$  

$ HERE COMES THE THERMODYNAMIC DATA (expressed in functions & parameters):  

$  

FUNCTION MGLIQUID 298.15 -4630.90976+192.994374*T-34.0888057*T*LOG(T)  

    -36544605.6*T**(-2); 6000 N!  

$  

FUNCTION MGSOLID 298.15 -8367.34+143.677876*T-26.1849785*T*LOG(T)  

    +4.858E-4*T**2-1.393669E-6*T**3+78950*T**(-1);  

    923.00 Y -13804.4772 +202.909445*T-34.0888057*T*LOG(T)  

    -3.65446056E7*T**(-2) +1.06753982E28*T**(-9); 6000 N!  

$  

FUNCTION SBLIQUID 298.15 9071.98+146.800*T-31.38*T*LOG(T)  

    -2.441646E8*T**(-2); 6000 N!  

$  

.....  

..... <more>  

$  

FUNCTION LFCT 298.15 -17325.6+5.03600*T; 6000 N!

```

---

```

FUNCTION GFCTSBSN 298.15 LFCT+SBSOLID+SNSOLID+2948.291+3721.286;
    6000 N!
FUNCTION ISB 298.15 15000; 6000 N!
FUNCTION ISN 298.15 47199.9-95.6270*T; 6000 N!
$
.....
..... <more>
$
PARAMETER G(RHOMBO,SB;0) 298.15 SBSOLID; 6000 N!
PARAMETER G(RHOMBO,SN;0) 298.15 2035+SNSOLID; 6000 N!
$
PARAMETER G(HCP,MG;0) 298.15 MGSOLID; 6000 N!
PARAMETER G(HCP,SN;0) 298.15 32000+SNSOLID; 6000 N!
PARAMETER G(HCP,MG,SN;0) 298.15 -69566-9.23183*T; 6000 N!
$
PARAMETER G(BCT,SN;0) 298.15 SNSOLID; 6000 N!
PARAMETER G(BCT,SB;0) 298.15 1000+SBSOLID; 6000 N!
PARAMETER G(BCT,SB,SN;0) 298.15 0.5*ISB+0.5*ISN; 6000 N!
PARAMETER G(BCT,SB,SN;1) 298.15 0.5*ISB-0.5*ISN; 6000 N!
$
PARAMETER G(IONICLIQ,MG2+:SB3-;0) 298.15 -204389-4.98506*T
    -2.75637E9*T**(-2)+3*MGLIQUID+2*SBLIQUID; 6000 N!
PARAMETER G(IONICLIQ,MG2+:SN4-;0) 298.15 -98639.5+881.073*T
    -174.523*T*LOG(T)-1.79808E9*T**(-2); 6000 N!
PARAMETER G(IONICLIQ,MG2+:SB;0) 298.15 SBLIQUID; 6000 N!
$
.....
..... <more>
$

```

### Example 3: A Public Database for the Fe-Cr-C Ternary System

```

$
$   Revision history:
$       Created as PDEMO   by Pingfang Shi   on 2004-10-05
$       Renamed to DFeCrC by Pingfang Shi   on 2006-10-25
$
$   FURTHER MODIFICATIONS:

```



---

```

        (only for demonstration purposes in TCC-Demo/TCW-Demo) '
*****
        (Version 1.2, Oct. 2006) ''

        Copyright © 2004-2012: Thermo-Calc Software AB, Sweden ''

The DFeCrC database (previously called PDEMO) is the TCS Demo Fe-Cr-C '
Alloy Solutions Database, which is especially designed for primarily '
demonstrating the uses of: '

    * TCC-Demo software: BIN, TERN, SCHEIL and some other modules; '

    * TCW-Demo software: '

        "Binary" module calculations of phase diagrams and property diagrams'
            in available binary systems; '

        "Ternary" module calculations of phase diagrams (e.g., isothermal'
            sections, monovariant lines involving liquid, liquidus'
            surface projections) and property diagrams in available'
            ternary systems; '

        "Scheil" module simulations of alloy solidifications; and/or '

        "Equilibrium" calculation routines for phase diagrams and property'
            diagrams in available binary or ternary systems. '

It can also be used for other types of calculations/simulations in both'
TCC and TCW software, and in their application programming interfaces.''

It includes critically-assessed data for all possible three binary joins'
(i.e. Cr-C, Fe-Cr and Fe-Cr) and one complete ternary alloy solutions '
within the Fe-Cr-C system. However, due to the fact that experimental'
data for the Fe-C and Cr-C binary joins and Fe-Cr-C ternary system at '
extremely-high temperatures are not sufficient, the available assessed'
data can not be applied to temperature conditions higher than 4000 K.''

Included thermodynamic data are available for various stoichiometric '
and solution phases, e.g. liquid mixture, various alloy solutions and '
intermetallic phases. But the gaseous mixture phase is excluded in this'
DEMO version.''

The DFeCrC database can be used not only in calculating various types '
of phase diagrams (binary phase diagrams, ternary isothermal sections,'
ternary monovariant lines involving liquid, ternary liquidus surface '
projections, ternary isopleth sections, etc.) and property diagrams '
(the easiest ways are through the BIN and TERN modules), but also in '
simulating alloy solidification processes (with the SCHEIL module) of'

```

---

!

VERSION DATE Last update and adjustment: Pingfang Shi, 2006-10-25 !

### \$ Definition of Elements in the Database System:

\$ELEM	NAME	STABLE	ELEMENT	REF	ATOMIC MASS	H298-H0	S298 !
--------	------	--------	---------	-----	-------------	---------	--------

\$-----

\$ELEMENT /-	ELECTRON GAS	0.0000E+00	0.0000E+00	0.0000E+00!
--------------	--------------	------------	------------	-------------

ELEMENT	VA	VACUUM	0.0000E+00	0.0000E+00	0.0000E+00!
---------	----	--------	------------	------------	-------------

ELEMENT C	GRAPHITE	1.2011E+01	1.0540E+03	5.7400E+00!
-----------	----------	------------	------------	-------------

ELEMENT	CR	BCC	A2	5.1996E+01	4.0500E+03	2.3560E+01!
---------	----	-----	----	------------	------------	-------------

ELEMENT	FE	BCC	A2	5.5847E+01	4.4890E+03	2.7280E+01!
---------	----	-----	----	------------	------------	-------------

[illegible]

\$ TYPE DEFINITIONS for data inclusions:

\$-----





---

```

FUNCT GFELIQ  298.15 +GHSEFE# +12040.17-6.55843*T
              -3.6751551E-21*T**7;  1811 Y
              -10839.7+291.302*T-46*T*LN(T);  6000 N!

FUNCT GFEFCC  298.15 +GHSEFE# -1462.4+8.282*T
              -1.15*T*LN(T)+6.4E-04*T**2;  1811 Y
              -27098.266+300.25256*T-46*T*LN(T)+2.78854E+31*T**(-9);  6000 N!

FUNCT GFCECM  298.15 +GPCEM1# -10745+706.04*T-120.6*T*LN(T);  6000 N!

FUNCT GFEM23C6  298.15 +7.666667*GFCECM#-1.666667*GHSECC#
              +66920-40*T;  6000 N!

FUNCT GCRFCC  298.15 +GHSERCR# +7284+.163*T;  6000 N!

FUNCT GCRM23C6  298.15 -521983+3622.24*T-620.965*T*LN(T)
              -.126431*T**2;  6000 N!

FUNCT GCRM3C2  298.15 -100823.8+530.66989*T-89.6694*T*LN(T)
              -.0301188*T**2;  6000 N!

FUNCT GCRM7C3  298.15 -201690+1103.128*T-190.177*T*LN(T)
              -.0578207*T**2;  6000 N!

FUNCT GPCLIQ  298.15 +YCLIQ#*EXP(ZCLIQ#);  6000 N!

FUNCT ACLIQ  298.15 +2.32E-05*T+2.85E-09*T**2;  6000 N!

FUNCT BCLIQ  298.15 +1+3.2E-10*P;  6000 N!

FUNCT CCLIQ  298.15 1.6E-10;  6000 N!

FUNCT DCLIQ  298.15 +1*LN(BCLIQ#);  6000 N!

FUNCT ECLIQ  298.15 +1*LN(CCLIQ#);  6000 N!

FUNCT VCLIQ  298.15 +7.626E-06*EXP(ACLIQ#);  6000 N!

FUNCT XCLIQ  298.15 +1*EXP(.5*DCLIQ#)-1;  6000 N!

FUNCT YCLIQ  298.15 +VCLIQ#*EXP(-ECLIQ#);  6000 N!

FUNCT ZCLIQ  298.15 +1*LN(XCLIQ#);  6000 N!

FUNCT GPCGRA  298.15 +YCGRA#*EXP(ZCGRA#);  6000 N!

FUNCT ACGRA  298.15 +2.32E-05*T+2.85E-09*T**2;  6000 N!

FUNCT BCGRA  298.15 +1+3.6E-10*P;  6000 N!

FUNCT CCGRA  298.15 3.3E-10;  6000 N!

FUNCT DCGRA  298.15 +1*LN(BCGRA#);  6000 N!

FUNCT ECGRA  298.15 +1*LN(CCGRA#);  6000 N!

```

---

---

```

FUNCT VCGRA      298.15 +5.259E-06*EXP(ACGRA#);      6000 N!
FUNCT XCGRA      298.15 +1*EXP(.9166667*DCGRA#)-1;    6000 N!
FUNCT YCGRA      298.15 +VCGRA#*EXP(-ECGRA#);        6000 N!
FUNCT ZCGRA      298.15 +1*LN(XCGRA#);                6000 N!

FUNCT GPCFCC     298.15 +YCFCC#*EXP(ZFEFCC#);        6000 N!
FUNCT ACFCC      298.15 +1.44E-04*T;                  6000 N!
FUNCT VCFCC      298.15 +1.031E-05*EXP(ACFCC#);        6000 N!
FUNCT YCFCC      298.15 +VCFCC#*EXP(-EFEFCC#);        6000 N!

FUNCT GPCRLIQ    298.15 +YCRLIQ#*EXP(ZCRLIQ#);        6000 N!
FUNCT ACRLIQ     298.15 +1.7E-05*T+9.2E-09*T**2;      6000 N!
FUNCT BCRLIQ     298.15 +1+4.65E-11*P;                6000 N!
FUNCT CCRLIQ     298.15 3.72E-11;                    6000 N!
FUNCT DCRLIQ     298.15 +1*LN(BCRLIQ#);                6000 N!
FUNCT ECRLIQ     298.15 +1*LN(CCRLIQ#);                6000 N!
FUNCT VCRLIQ     298.15 +7.653E-06*EXP(ACRLIQ#);      6000 N!
FUNCT XCRLIQ     298.15 +1*EXP(.8*DCRLIQ#)-1;         6000 N!
FUNCT YCRLIQ     298.15 +VCRLIQ#*EXP(-ECRLIQ#);        6000 N!
FUNCT ZCRLIQ     298.15 +1*LN(XCRLIQ#);                6000 N!

FUNCT GPCRBCC    298.15 +YCRBCC#*EXP(ZCRBCC#);        6000 N!
FUNCT ACRBCC     298.15 +1.7E-05*T+9.2E-09*T**2;      6000 N!
FUNCT BCRBCC     298.15 +1+2.6E-11*P;                6000 N!
FUNCT CCRBCC     298.15 2.08E-11;                    6000 N!
FUNCT DCRBCC     298.15 +1*LN(BCRBCC#);                6000 N!
FUNCT ECRBCC     298.15 +1*LN(CCRBCC#);                6000 N!
FUNCT VCRBCC     298.15 +7.188E-06*EXP(ACRBCC#);      6000 N!
FUNCT XCRBCC     298.15 +1*EXP(.8*DCRBCC#)-1;         6000 N!
FUNCT YCRBCC     298.15 +VCRBCC#*EXP(-ECRBCC#);        6000 N!
FUNCT ZCRBCC     298.15 +1*LN(XCRBCC#);                6000 N!

FUNCT GPFELIQ    298.15 +YFELIQ#*EXP(ZFELIQ#);        6000 N!
FUNCT AFELIQ     298.15 +1.135E-04*T;                  6000 N!
FUNCT BFELIQ     298.15 +1+4.98009787E-12*P+3.20078924E-14*T*P; 6000 N!
FUNCT CFELIQ     298.15 +4.22534787E-12+2.71569924E-14*T; 6000 N!

```

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```

FUNCT DFELIQ 298.15 +1*LN(BFELIQ#); 6000 N!
FUNCT EFELIQ 298.15 +1*LN(CFELIQ#); 6000 N!
FUNCT VFELIQ 298.15 +6.46677E-06*EXP(AFELIQ#); 6000 N!
FUNCT XFELIQ 298.15 +1*EXP(.8484467*DFELIQ#)-1; 6000 N!
FUNCT YFELIQ 298.15 +VFELIQ#*EXP(-EFELIQ#); 6000 N!
FUNCT ZFELIQ 298.15 +1*LN(XFELIQ#); 6000 N!

FUNCT GPFEFCC 298.15 +YFEFCC#*EXP(ZFEFCC#); 6000 N!
FUNCT AFEFCC 298.15 +7.3097E-05*T; 6000 N!
FUNCT BFEFCC 298.15 +1+3.25236341E-11*P+3.36607808E-16*T*P; 6000 N!
FUNCT CFEFCC 298.15 +2.62285341E-11+2.71455808E-16*T; 6000 N!
FUNCT DFEFCC 298.15 +1*LN(BFEFCC#); 6000 N!
FUNCT EFEFCC 298.15 +1*LN(CFEFCC#); 6000 N!
FUNCT VFEFCC 298.15 +6.688726E-06*EXP(AFEFCC#); 6000 N!
FUNCT XFEFCC 298.15 +1*EXP(.8064454*DFEFCC#)-1; 6000 N!
FUNCT YFEFCC 298.15 +VFEFCC#*EXP(-EFEFCC#); 6000 N!
FUNCT ZFEFCC 298.15 +1*LN(XFEFCC#); 6000 N!

FUNCT GPFEBC 298.15 +YFEBCC#*EXP(ZFEBCC#); 6000 N!
FUNCT AFEBC 298.15 +2.3987E-05*T+1.2845E-08*T**2; 6000 N!
FUNCT BFEBC 298.15 +1+2.80599565E-11*P+3.06481523E-16*T*P; 6000 N!
FUNCT CFEBCC 298.15 +2.20949565E-11+2.41329523E-16*T; 6000 N!
FUNCT DFEBCC 298.15 +1*LN(BFEBC#); 6000 N!
FUNCT EFEBCC 298.15 +1*LN(CFEBCC#); 6000 N!
FUNCT VFEBCC 298.15 +7.042095E-06*EXP(AFEBC#); 6000 N!
FUNCT XFEBCC 298.15 +1*EXP(.7874195*DFEBCC#)-1; 6000 N!
FUNCT YFEBCC 298.15 +VFEBCC#*EXP(-EFEBCC#); 6000 N!
FUNCT ZFEBCC 298.15 +1*LN(XFEBCC#); 6000 N!

FUNCT GPFEHCP 298.15 +YFEHCP#*EXP(ZFEHCP#); 6000 N!
FUNCT AFEHCP 298.15 +7.3646E-5*T; 6000 N!
FUNCT BFEHCP 298.15 +1+32.5236341E-12*P+3.36607808E-16*P*T; 6000 N!
FUNCT CFEHCP 298.15 +26.2285341E-12+2.71455808E-16*T; 6000 N!
FUNCT DFEHCP 298.15 +LOG(BFEHCP#); 6000 N!
FUNCT EFEHCP 298.15 +LOG(CFEHCP#); 6000 N!
FUNCT VFEHCP 298.15 +6.59121E-6*EXP(AFEHCP#); 6000 N!

```

---



---

```

PARAM L (LIQUID,C,FE;1) 298.15 +19300; 6000 N REF3 !
PARAM L (LIQUID,C,FE;2) 298.15 +49260-19*T; 6000 N REF3 !
PARAM L (LIQUID,CR,FE;0) 298.15 -14550+6.65*T; 6000 N REF4 !
PARAM L (LIQUID,C,CR,FE;0) 298.15 -496063; 6000 N REF2 !
PARAM L (LIQUID,C,CR,FE;1) 298.15 +57990; 6000 N REF2 !
PARAM L (LIQUID,C,CR,FE;2) 298.15 +61404; 6000 N REF2 !

$***** FCC_A1 (Solution) *****
$PHASE FCC_A1 %BC 2 1 1 !
$ Note the C TYPE_DEF for 2nd FCC composition-set (MC) is not necessary
$ for the (Fe,Cr)-C system.
PHASE FCC_A1 %B 2 1 1 !
CONST FCC_A1 : CR,FE%
: C,VA% : !

PARAM G (FCC_A1,CR:VA;0) 298.15 +GCRFCC#+GPCRBCC#; 6000 N REF0 !
PARAM TC (FCC_A1,CR:VA;0) 298.15 -1109; 6000 N REF0 !
PARAM BMAGN (FCC_A1,CR:VA;0) 298.15 -2.46; 6000 N REF0 !
PARAM G (FCC_A1,FE:VA;0) 298.15 +GFEFCC#+GPFEFCC#; 6000 N REF0 !
PARAM TC (FCC_A1,FE:VA;0) 298.15 -201; 6000 N REF0 !
PARAM BMAGN (FCC_A1,FE:VA;0) 298.15 -2.1; 6000 N REF0 !

PARAM G (FCC_A1,CR:C;0) 298.15 +GHSERCR#+GHSERCC#
+1200-1.94*T; 6000 N REF2 !
PARAM G (FCC_A1,FE:C;0) 298.15 +GFEFCC#+GHSERCC#+GPCFCC#
+77207-15.877*T; 6000 N REF3 !
PARAM TC (FCC_A1,FE:C;0) 298.15 -201; 6000 N REF3 !
PARAM BMAGN (FCC_A1,FE:C;0) 298.15 -2.1; 6000 N REF3 !

PARAM L (FCC_A1,CR:C,VA;0) 298.15 -11977+6.8194*T; 6000 N REF2 !
PARAM L (FCC_A1,FE:C,VA;0) 298.15 -34671; 6000 N REF3 !
PARAM L (FCC_A1,CR,FE:VA;0) 298.15 +10833-7.477*T; 6000 N REF4 !
PARAM L (FCC_A1,CR,FE:VA;1) 298.15 +1410; 6000 N REF4 !
PARAM L (FCC_A1,CR,FE:C;0) 298.15 -74319+3.2353*T; 6000 N REF2 !

$***** BCC_A2 (Solution) *****

```

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---

```

PHASE BCC_A2  %A  2 1  3 !
CONST BCC_A2  : CR%,FE%
              : C,VA% :  !

PARAM G(BCC_A2,CR:VA;0)  298.15 +GHSERCR#+GPCRBCC#;  6000 N REF0 !
PARAM TC(BCC_A2,CR:VA;0)      298.15 -311.5;  6000 N REF0 !
PARAM BMAGN(BCC_A2,CR:VA;0)  298.15  -.01;  6000 N REF0 !
PARAM G(BCC_A2,FE:VA;0)  298.15 +GHSEFFE#+GPFEBCC#;  6000 N REF0 !
PARAM TC(BCC_A2,FE:VA;0)      298.15 1043;  6000 N REF0 !
PARAM BMAGN(BCC_A2,FE:VA;0)  298.15 2.22;  6000 N REF0 !

PARAM G(BCC_A2,CR:C;0)  298.15 +GHSERCR#+3*GHSEGCC#+GPCRBCC#+3*GPCGRA#
                        +416000;  6000 N REF1 !
PARAM TC(BCC_A2,CR:C;0)      298.15 -311.5;  6000 N REF1 !
PARAM BMAGN(BCC_A2,CR:C;0)  298.15  -.008;  6000 N REF1 !
PARAM G(BCC_A2,FE:C;0)  298.15 +GHSEFFE#+3*GHSEGCC#+GPFEBCC#+3*GPCGRA#
                        +322050+75.667*T;  6000 N REF3 !
PARAM TC(BCC_A2,FE:C;0)      298.15 1043;  6000 N REF3 !
PARAM BMAGN(BCC_A2,FE:C;0)  298.15 2.22;  6000 N REF3 !

$ PF-20061025: Modify the L(BCC_A2,FE:C,VA;0) [and L(BCC_A2,CR:C,VA;0)]
$      parametera, in order to avoid BCC-appearance (Fe-C)
$      at temperatures higher than 3900 K.

$PARAM L(BCC_A2,CR:C,VA;0)  298.15 -190*T;  6000 N REF1 !
PARAM L(BCC_A2,CR:C,VA;0)  298.15 -190*T; 3000 Y 0; 6000 N REFS !
$PARAM L(BCC_A2,FE:C,VA;0)  298.15 -190*T;  6000 N REF3 !
PARAM L(BCC_A2,FE:C,VA;0)  298.15 -190*T; 3900 Y 0; 6000 N REFS !
$

PARAM L(BCC_A2,CR,FE:VA;0)  298.15 +20500-9.68*T;  6000 N REF4 !
PARAM TC(BCC_A2,CR,FE:VA;0)      298.15 1650;  6000 N REF4 !
PARAM TC(BCC_A2,CR,FE:VA;1)      298.15  550;  6000 N REF4 !
PARAM BMAGN(BCC_A2,CR,FE:VA;0)  298.15  -.85;  6000 N REF4 !

PARAM L(BCC_A2,CR,FE:C;0)  298.15 -1250000+667.7*T; 6000 N REF2 !
PARAM TC(BCC_A2,CR,FE:C;0)      298.15 1650;  6000 N REF5 !
PARAM TC(BCC_A2,CR,FE:C;1)      298.15  550;  6000 N REF5 !

```

---

---

```

PARAM BMAGN(BCC_A2,CR,FE:C;0) 298.15 -.85; 6000 N REF5 !

$***** HCP_A3 (Solution) *****
$PHASE HCP_A3 %BC 2 1 .5 !
$ Note the C TYPE_DEF for 2nd HCP composition-set (M2C) is not necessary
$ for the (Fe,Cr)-C system.
PHASE HCP_A3 %B 2 1 .5 !
CONST HCP_A3 : CR,FE,
               : VA%,C : !

PARAM G(HCP_A3,CR:VA;0) 298.15 +GHSERCR#+4438; 6000 N REF1 !
PARAM TC(HCP_A3,CR:VA;0) 298.15 -1109; 6000 N REF1 !
PARAM BMAGN(HCP_A3,CR:VA;0) 298.15 -2.46; 6000 N REF1 !
PARAM G(HCP_A3,FE:VA;0) 298.15 +GHSEFFE#+GPFEHCP#
                        -3705.78+12.591*T-1.15*T*LN(T)+6.4E-04*T**2; 1811 Y
                        +GHSEFFE#+GPFEHCP#
                        -3957.199+5.24951*T+4.9251E+30*T**(-9); 6000 N REF0 !
PARAM G(HCP_A3,CR:C;0) 298.15 +GHSERCR#+.5*GHSEGCC#
                        -18504+9.4173*T-2.4997*T*LN(T)+.001386*T**2; 6000 N REF1 !
PARAM G(HCP_A3,FE:C;0) 298.15 +GFEFCC#+.5*GHSEGCC#+GPCFCC#
                        +52905-11.9075*T; 6000 N REF3 !

PARAM L(HCP_A3,CR:C,VA;0) 298.15 +4165; 6000 N REF1 !
PARAM L(HCP_A3,FE:C,VA;0) 298.15 -22126; 6000 N REF3 !
$PARAM L(HCP_A3,FE:C,VA;0) 298.15 -17335; 6000 N TCFE3 !
PARAM L(HCP_A3,CR,FE:VA;0) 298.15 +10833-7.477*T; 6000 N REF4 !

$***** SIGMA (Solution) *****
PHASE SIGMA % 3 8 4 18 !
CONST SIGMA : FE
              : CR
              : CR,FE : !

PARAM G(SIGMA,FE:CR:CR;0) 298.15 +8*GFEFCC#+22*GHSERCR#
                        +92300-95.96*T+GPSIG1#; 6000 N REF4 !
PARAM G(SIGMA,FE:CR:FE;0) 298.15 +8*GFEFCC#+4*GHSERCR#+18*GHSEFFE#

```

---

---

+117300-95.96\*T+GPSIG2#; 6000 N REF4 !

\$\*\*\*\*\* CEMENTITE (Solution) \*\*\*\*\*

PHASE CEMENTITE % 2 3 1 !

CONST CEMENTITE : CR,FE%

: C : !

PARAM G (CEMENTITE,CR:C;0) 298.15 +3\*GHSERCR#+GHSERCC#

-48000-9.2888\*T; 6000 N REF2 !

PARAM G (CEMENTITE,FE:C;0) 298.15 +GFECCEM#; 6000 N REF3 !

PARAM L (CEMENTITE,CR,FE:C;0) 298.15 +25278-17.5\*T; 6000 N REF2 !

\$\*\*\*\*\* M3C2 (Compound) \*\*\*\*\*

PHASE M3C2 % 2 3 2 !

CONST M3C2 : CR

: C : !

PARAM G (M3C2,CR:C;0) 298.15 +GCRM3C2#; 6000 N REF2 !

\$\*\*\*\*\* M7C3 (Solution) \*\*\*\*\*

PHASE M7C3 % 2 7 3 !

CONST M7C3 : CR%,FE

: C : !

PARAM G (M7C3,CR:C;0) 298.15 +GCRM7C3#; 6000 N REF2 !

PARAM G (M7C3,FE:C;0) 298.15 +7\*GHSERFE#+3\*GHSERCC#

+75000-48.2168\*T; 6000 N REF2 !

PARAM L (M7C3,CR,FE:C;0) 298.15 -4520-10\*T; 6000 N REF2 !

\$\*\*\*\*\* M23C6 (Solution) \*\*\*\*\*

PHASE M23C6 % 3 20 3 6 !

CONST M23C6 : CR%,FE%

: CR%,FE%

: C : !

---





```
!  
  
$  
$  
$  
$  
$ LIST OF REFERENCE:  
$  
$-----  
LIST_OF_REFERENCES  
NUMBER SOURCE  
REF0 'Alan Dinsdale, SGTE Data for Pure Elements, Calphad Vol 15 (1991)  
      p 317-425, also in NPL Report DMA(A)195 Rev. August 1990'  
REF1 'J-O Andersson, Calphad Vol 11 (1987) p 271-276, TRITA 0314; C-CR'  
REF2 'Byeong-Joo Lee, unpublished revision (1991); C-Cr-Fe-Ni'  
REF3 'P. Gustafson, Scan. J. Metall. vol 14, (1985) p 259-267  
      TRITA 0237 (1984); C-FE'  
REF4 'J-O Andersson, B. Sundman, CALPHAD Vol 11, (1987), p 83-92  
      TRITA 0270 (1986); CR-FE'  
REF5 'J-O Andersson, Met. Trans A, Vol 19A, (1988) p 627-636  
      TRITA 0207 (1986); C-CR-FE'  
REFS 'Pingfang Shi (2006), TCS PTERN Public Ternary Alloys Database,  
      v1.2; Modified L0 (BCC,Fe,C) and L0 (BCC,Cr,C) parameters  
      at high temperatures.'  
!
```

---

# The Database Checker

In this section:

---

<i>About the Database Checker .....</i>	<i>65</i>
<i>Database Checker Revision History .....</i>	<i>65</i>

## About the Database Checker

The Thermo-Calc software package includes a program to check that the syntax of unencrypted database files is correct. The program applies the syntax rules set out in the *Database Manager User Guide* and reports errors and issues warnings. This program is intended for advanced users who develop and manage databases.



Thermo-Calc accepts deviations from these syntax rules. This means that a database can work even if the Database Checker reports errors and warnings. For example, an error is reported if an abbreviated phase name is found, but phase name abbreviations are accepted by Thermo-Calc and its add-on modules.

The executable **DatabaseChecker** file is found in the Thermo-Calc home directory. The program can also be launched by selecting **Tools→ Database Checker** from the main menu.



[Database Checker Revision History](#) below for releases notes that may assist database developers.

## Database Checker Revision History

The DatabaseChecker application is standalone and need not be installed separately, just download the containing zip file, open it and follow the instructions in the README.TXT file. The program requires that Java is installed on the target machine. Please note that large amounts of RAM may be required when checking large databases.

## Release Notes Version 1.4

- The DatabaseChecker user interface has been modified to allow checking of several database files in one batch. Instead of selecting an individual database file, the user now selects a directory that contains databases. The application then shows a tree structure with all database files in the chosen directory and its subdirectories. The user may then select any number of these files for processing.
- A check of parameters whose interaction order is 3 has been introduced. For such parameters, there must either exist one parameter with the interaction degree 0 or three parameters with the interaction degrees 0, 1 and 2.
- To facilitate optimization of databases, the tool now generates information messages about functions and parameters that will always return 0.

## Release Notes, Version 1.3.2

- The tool now detects conflicts between identical parameters even if one of them have been defined with the G prefix and the other with the L prefix.

## Release Notes, Version 1.3

A bug prevented integers bigger than 32 bits from being parsed. This has been corrected.

The tool now checks that the species and number of sublattices used in parameter definitions match the phase definition and generates an error message for every mismatch. Ionic liquid parameters are currently exempted from this check as not to break the widespread use of defining only one constituent for ionic liquid parameters.

Type definitions and case statements are now parsed for errors. However, only a subset of all possible GES, POLY and TDB commands are accepted and all other commands will result in an error message. The accepted commands are:

- GES AMEND\_PHASE\_DESCRIPTION
- COMPOSITION\_SETS
- MAJOR\_CONSTITUENTS
- DISORDERED\_PART
- MAGNETIC\_ORDERING
- STATUS\_BITS
- DEFAULT\_STABLE
- FRACTION\_LIMITS
- EXCESS\_MODEL

- 
- REDLICH-KISTER\_MUGGIANU
  - HKF
  - HKF\_ELECTROSTATIC
  - DEBYE\_HUCKEL
  - GES CHANGE\_STATUS
  - TDB DEFINE\_SYSTEM\_ELEMENTS
  - TDB RESTORE\_PHASES
  - TDB REJECT\_PHASES

Some improvements to warning and error messages have been made to facilitate finding errors.

### Release Notes, Version 1.2

- The tool now uses parallel processing of database files on multi-core systems. This significantly improves performance when large databases are checked.
- It is no longer required that inter-dependent database statements are defined in a specific order in the database file (e.g., species need not any longer be defined before the elements on which they depend). However, for the sake of readability, it is still advised that the database statements occur in a natural order in the file.
- Because of the parallel processing of database statements, multiple definition errors (cases where one name has been used to define more than one entity in the database e.g, two identically named species) may now be generated for any of the violating occurrences and not only for the last occurrence in the file.

### Release Notes, Version 1.1

- Phase names were not properly recognized in parameter definitions if there was one or more whitespace characters between the opening parenthesis and the phase name. This has been corrected.
- The error message Could not parse parameter, <species name> has been given without a sublattice number but is defined in more than one sublattice is now displayed only for phases where the general diffusion model is used. Note: this implementation is temporary and may be subject to changes later.
- The meaning of the information message The phase <phase name> expects the following parameters: [<parameter names>] was unclear to users. It is now longer shown for the parameter names T and P. For all other names, the message is now displayed as an error message with the following text: The phase <phase name> contains references to the following undefined functions: [<function names>].

- The tool now looks for function names that are abbreviations of other function names and warns about this, since abbreviated names may cause problems during the execution of macro files that have been auto-generated from GES.
- The tools also warns for functions whose names are in the format V<integer>, since this may cause conflicts with names that are used by PARROT.
- Parameter names are now shown in a format that is less cryptic and more resembles the format used in the database. However, the format of diffusion parameters may still differ somewhat from what is used in the database.

### Release Notes, Version 1.0

- The tool parses a TDB file and produces a log with error, warning and information messages about the state of the file
- The message log can be exported and saved as a separate file for later analysis
- The tool is based on the database command definitions given in TC\_Database\_ManagersGuide and DICTRA27\_UsersGuide. All commands in these documents are supported. Some undocumented DIFFUSION commands are not supported.
- Databases that span several files are correctly handled, also blocked files
- The tool is in some aspects more strict than required by the guides (see Additional Information below)
- The tool performs the following checks:
  - Syntax control of database statements: ERROR
  - Line size: ERROR or WARNING depending on context
  - Multiply defined elements, species or phases: ERROR
  - Multiply defined functions and parameters: ERROR
  - Multiply defined assessed system: ERROR
  - Multiply defined references: ERROR
  - References entries that are never used: WARNING
  - References to non-existent type definitions: ERROR
  - Type definitions that are never used: WARNING
  - Unused functions and parameters: WARNING
  - Functions and parameters with undefined references: WARNING
  - References to undefined elements, species or phases: ERROR

- Dependencies to external names from a phase: INFORMATION. (All parameters of a phase are evaluated with respect to their dependencies to other parameters and functions and all unresolved names are listed. Typically, this should only yield dependencies on T and possibly P)

### Additional Information

In addition to the command definitions given in the user guides listed above, the following rules are also applied:

- Names are case-sensitive, meaning that e.g., the defined element MN cannot be referred to under the name Mn;
- Phase names cannot be abbreviated. When referred to in parameter descriptions their full names must be used.



# Index

---

## 2

2SL model 63

## 4

4SL model 61-62

## A

A phase 67

abbreviations

    command names 120

about the software 240

activities 4, 20

activity 28

activity curves 106

activity nodes 28

    descriptions 34

add new components

    installations 23

add\_comment 43

add\_constituent 15

add\_initial\_equilibrium 119

add\_label\_text 191

add\_reference 37

advanced mode 75

advanced\_options 120, 125

allotropic\_phase 16

alloy definition 31

alloy solution phase 10

alternate mode 28, 43-44

amend\_element\_data 43

amend\_parameter 44, 88

amend\_phase\_description 53

amend\_selection 12

amend\_stored\_equilibria 133

amend\_symbol 58, 91

append project 33

append\_database 13

append\_experimental\_data 183, 193, 38, 11

AQS 163

aqueous solution phase 283, 10-11

aqueous solutions 162, 3, 7

assessed\_system 32

atomistic properties 57

attribute command 20

    DATAPLOT 10

auxiliary text string 13

axis variable 90

## B

B phase 67

back command 4

background color 203

bcc\_to\_fcc\_transformation 236

binary calculator 104

---

binary equilibrium 21  
binary systems 51  
binary\_diagram 10  
block command 7, 19  
blockend 20  
blocks 15  
border width 201  
buffer size 203

## C

calculate an equilibrium 134  
calculating a potential diagram 158  
calculation mode 195  
calorimetric data 53-54  
CALPHAD 4  
    database 70  
caption style 201  
case 38  
change\_legend 194  
change\_status 60, 135  
charsize 22  
check for update 34  
client computer 5  
clip command 20  
    DATAPLOT 10  
clones 47-48  
close 127  
close\_file 240

---

coarsening model 70  
color codes, DATAPLOT 22, 41  
command history 123  
command line prompt 119  
command names  
    entering 120  
comment command 41, 21  
compile\_experiments 93, 29  
complex alloys  
    Pourbaix diagrams 21  
composition sets 26, 62  
composition\_sets 47  
compositional extensive variables 273  
Compound Energy Formalism (CEF) 60  
compound solution phase 10  
compound\_phase 16  
compute\_all\_equilibria 23  
compute\_equilibrium 140  
compute\_transition 141  
computing equilibria 32  
conditions tab 73  
configuration window 46  
console  
    name 203  
    output 123  
    results window 116  
    window 113

---

console mode 4, 112

examples 14

settings 203

visualisation 180

consolidated network installations 5, 9

constituent

array 63, 98

description 15

constituents 67, 14

constitutional composition-related extensive  
variable 275

context help 6

continue\_optimization 94

coordinate systems 5

corrosion 3

create\_dividers 229

create\_new\_equilibrium 143

create\_new\_store\_file 94

create\_pipes 229

create\_stage\_boxes 230

critical set of experiments 34

crosshair 95

crystal structures 56

curves 33

custom network client installation 33

custom standalone installations 23

---

## D

data-type code 13

data forms 190

DATA module 3, 9

data optimization 3

data optimization workflow 7

data points 202

data sets

optimization 49

database

definition 7

directory 188

file 40-41

initiation file 3, 41

packages 192

selection 191

database checker 16, 33, 186, 65

database directory file 17

database initiation file 17

database\_information 13, 18

DATAPLOT 104, 38, 3

datapoint 20

dataset 5, 19

debugging 51

Debye\_Huckel 51

decimal digits 199

---

default directory 203  
     installation 13  
 default units 189  
 default\_command 17  
 default\_stable 52  
 define\_components 144, 15  
 define\_diagram 145  
 define\_elements 14  
 define\_material 147  
 define\_species 14  
 define\_system 15  
 define\_system\_default 16  
 defining a system 127  
 delete\_initial\_equilibrium 151  
 delete\_symbol 151  
 derived variables 190, 281  
 DGM condition 22  
 diagram\_type 17  
 diffusion 43  
 DIGLIB 11  
 disk-based cache. 185  
 disordered phase 69  
 disordered\_part 48  
 display color 200  
 display\_license\_info 127, 240  
 distributed network installations 5, 10  
 DOP file 37

---

dormant phase 134  
 drag and drop labels 94  
 drawline 8, 21  
 driving force 140, 22, 55  
 driving force for metastable phases 195  
 driving force model 69  
 dump\_diagram 194

## E

ED\_EXP 31  
     module 7  
 edit\_experiments 23, 95, 8  
 effective interaction ratio 5  
 element 7  
 element name 8  
 EMF measurements 55  
 empty reference 37  
 endcase 38  
 energy-related extensive variables 272  
 enter\_element 61  
 enter\_function 246  
 enter\_parameter 65, 99  
 enter\_phase 70  
     about 67  
 enter\_reaction 248  
 enter\_species 72  
 enter\_symbol  
     GES module 73

---

---

POLY and POST modules 153, 196

EOS 56

equation of state data 56

equilibria

    computing 32

equilibrium 133, 17

equilibrium calculations 131, 134

equilibrium calculator 72-73, 194

equilibrium model 72

equilibrium\_calculator 120

evaluate\_functions 155

evaluate\_segration\_profile 236

event log window 51, 116, 189

example projects 7

examples

    Graphical Mode 9

excess Gibbs energy terms 65

excess\_model 49

execute\_poly3\_command 231

exit command 4

EXP-file 10

experiment 25

experiment command 19

experimental data files 24, 37

experimental file reader 104

export 27

---

## F

F phase 67

file menu 127

file types 2

    console mode 123

find\_line 198

fixed phase 134

    equilibrium calculation 75

flush\_buffer 41, 15

font command 24

    DATAPLOT 8

fonts 201, 203

FORTTRAN 22

four substitutional-sublattice ordering  
    model 68, 12

fraction\_limits 48

FTP\_file 21

functions 76, 283, 27

    analytical 8

    keyword 22

## G

G parameters 68

G phase 67

gas phase 11, 16

gaseous mixture phase 60, 10

Gaussian distribution 65, 4

GES5 file 83

---

get\_data 16

Gibbs energy 3, 26

Gibbs energy curves 106

GIBBS module 47, 8, 17

GIBBS parameter name 25

GIBBS parameters 42

GIBBS phase-type codes 10

GIBBS phase rule 131

glass\_transition 52

global minimization 131, 195

global settings

    appearance 203

    calculation 194

    general 188

    graphical mode 190

    plotting 200

    scheil 198

    system definition 191

    tabulation 199

global\_minimization 120, 236

globalsize 22

GOC 6

goto\_module 4

graphical files 190

graphical mode 4, 27, 189

    examples 9

    settings 190

---

workflow 32

graphical operation code 5

grid points 195

GUI language 188

GUI layout 27, 188

## H

help 33

    console mode 6

help commands 5

Hessian matrix 94

heterogeneous equilibrium 6

heterogeneous interaction systems 22

heterogeneous interactions 5, 7

hkf\_electrostatic 51

host ID 5

hp\_calculator 241

## I

I2SL model 61

immunity 3

import 28

in-memory cache 185

include command

    DATAPLOT 10, 28

information command 5

installation requirements 3

installation types 8

---

---

intensive variables 271

interaction parameters 27

interaction\_parameter 63, 98

interfacial energy model 70

invariant equilibria 49

ionic two-sublattice liquid (I2SL) model 61

ionic two sublattice liquid (I2SL) model 26

ionic\_liq 26

isothermal section 108

## K

keywords 7

kinetic data 42

kinetic database 3

## L

label an equilibrium 22

label format 201

label text 92

label\_data 28

LaTeX 93, 182, 9, 11-12

lattice stability 44

least-squares method 4

legend option and style 89

legend styles 91

libgfortran 4.4 18

license errors

troubleshooting 45

---

license files 5, 38

license information 23

license keys 5, 8

requesting 38

License Manager (Windows) 5

installation 28

license server 5

License Server (Linux) 5

licenses 8, 23

licensing software 5

limits 90

line types

DATAPLOT 10, 32

line width and type 202

lines

DATAPLOT 30

linetype 21

Linux installations 8

Linux License Server installations 29

liquid phase 60

liquid\_phase\_name 237

liquidus projection 108

list\_all\_equilibria 28

list\_all\_variables 101

list\_axis\_variable 155

list\_conditions 102, 156

list\_constituent 77

---

---

list\_data 78

list\_data\_table 199

list\_database 16

list\_equilibrium 156

list\_initial\_equilibria 157

list\_of\_reference 36

list\_parameter 79, 103

list\_phase\_addition 122

list\_phase\_data 80, 104

list\_plot\_settings 199

list\_records 231

list\_result 104

list\_status 80, 157

list\_store\_file 108

list\_substances 249

list\_symbol 83

list\_symbol\_in\_ges 109

list\_symbols 158, 199

list\_system 16

load\_initial\_equilibrium 158

log files 124

LTEXT 182, 13

## M

Mac installations 8

macro files 7, 14, 124, 9, 38

macro\_file\_open 6

magnetic ordering 64

---

magnetic\_ordering 49

main menu 32

major\_constituent 47, 122

make\_experimental\_datafile 200

make\_pop\_file 29

map 158

maximize windows 39

meshing points 196

metal-aqueous interaction system 3

metastable equilibria 135

metastable phases 55

metastable states 49

minimize windows 39

modify\_label\_text 200

modifying diagrams 181

modules 5, 20, 119

molar volumes 64

monovariant lines 108

move activities 39

moving windows 39

MS-Excel 198

multi-user network installations 9

my project node 36

## N

network computer installation 27, 24

Network License (NWL) 6

new 32



---

new\_composition\_set 122

new\_constituent 47

new\_directory\_file 17

nodes 28

normal 4-sublattice model 67, 11

normalized coordinate system 5

normalizing suffixes 276

number format 199

NWL 10

## O

online help 5, 33

OPCODEs 241

open 32

open files 127

open\_file 241

optimization 37, 7, 26

    conflicting data and 49

optimization guidelines 48

optimization workflow 31

optimize\_variables 109, 34

optimizing 43

options 33

    keyword 31

order-disorder transformations 61

ordered phase 69

ordered phase with disordered  
    contribution 21

---

output\_file\_for\_show 122

## P

paint command 27

    DATAPLOT 8

PAQ and PAQS databases 10

paraequilibrium 154, 122

parameter keyword 24, 42

parameter name 62, 79, 96, 103

PARROT module 37, 7, 26, 31

PARROT workspace file 29

partial derivatives 281

passivity 3

pcfunction 27

perform tree 49

pH-Eh phase diagram 162

pH-Eh plot 5

phase

    boundaries 3

    boundary lines 139

    keyword 9

    name 63, 98, 9, 14

phase diagram 141-142, 51

    binary calculator 106

    plotting 38

phase fractions 106

phase names 67

phase stability function 22

---

- 
- phase transition model 68
  - phase types 67
  - phase\_addition 123
  - plot
    - labels 92
    - properties 95, 200
    - several calculations 96
    - type 89
  - plot a diagram 180
  - plot renderer 76, 83
  - plot\_diagram 201
  - POLY module 117
  - POLY3 calculations 8
  - POLY3 workspace file 165
  - polygons 8
    - DATAPLOT 31
  - POP-file 14, 22, 29, 31, 55
  - POP file 37, 9, 29, 31
  - post 160
  - POST module 181, 190
  - potential diagram 159
  - potential module 158
  - potential phase diagram 158
  - potential\_diagram 218
  - Pourbaix diagrams 162-163, 165, 167, 220, 3, 5, 10, 16, 19, 22
  - POURBAIX module 165
  - precipitation of a phase 22
  - predecessor 28
  - predecessors 31
  - present\_phase 123
  - print\_diagram 201
  - printing 123
  - project 28
  - project activity nodes 34
  - project files
    - open 9
    - opening 34
  - project window 40, 46, 49
  - prologue 5, 11, 15
  - property diagrams 137, 139
    - plotting 38
  - property model calculator 60, 64, 68-72
    - workflow 61
- Q**
- quantity relation 24
  - quasi-binary phase diagram 142
  - quasi-ternary phase diagram 143
  - quasichem\_fact00 52
  - quasichem\_ionic 51
  - quasichem\_irsid 52
  - quick start wizard 43
  - quick\_experimental\_plot 183, 202, 11
-

---

**R**

read command 29  
read\_ges\_workspace 83  
read\_parrot\_workspace 109  
read\_workspace 232  
read\_workspaces 126, 160  
recover\_start\_values 160  
recover\_variables 110  
Redlich-Kister-Muggianu model 65  
Redlich-Kister expression 27  
redox reactions 16  
ref\_electrode 10  
reference state type 17  
reference\_file 35  
reinitiate 84, 110  
reinitiate\_module 161  
reinitiate\_plot\_settings 202  
reject 18  
relative standard deviation (RSD) 36  
remove\_addition 52  
rename\_phase 47  
rescale\_variables 110  
reset windows 38  
response-driven module 126-127  
restore 19  
restore\_all\_weights 30  
restore\_phase\_in\_plot 202

---

results tab 116

retain labels 88, 201

rotation angle 94

rounding off variables 40-41

**S**

save 33

diagram 88

diagrams 183

plots 95

project files 34

workspace 127

save\_file\_name 237

save\_ges\_workspace 85

save\_parrot\_workspace 111

save\_workspace 232

save\_workspaces 126, 30, 162, 15

scheduler 40, 49

Scheil-Gulliver solidification 108, 145-146

Scheil calculator 108, 198

Scheil simulation diagrams 148

secondary keyword and parameters 17

secondary keywords, type-definition com-  
mand 18

secondary solid phase 10

select nodes 39

select\_equilibrium 162

select\_plot 202

---

---

SER 43	set_numerical_limits 169
server network installations 10	set_optimizing_condition 113
set_all_start_values 162	set_optimizing_variable 114
set_alterate_condition 31	set_output_levels 115
set_alterate_mode 111	set_plot_environment 243
set_auto_append_database 20	set_plot_format 211, 251
set_axis_length 203	set_plot_options 211
set_axis_plot_status 203	set_plot_size 213
set_axis_text_status 203	set_prefix_scaling 213
set_axis_type 204	set_r_and_p_norm 85
set_axis_variable 164	set_raster_status 213
set_color 204	set_reference_state 143, 170, 214
set_command_unit 241	set_scaled_variable 116
set_condition 143, 166	set_scaling_status 214
set_corner_text 206	set_start_constitution 171
set_diagram_axis 207	set_start_value 172
set_diagram_type 208	set_store_file 116
set_echo 242	set_tc_options 244
set_energy_unit 251	set_tic_type 215
set_external_parameter 112	set_tieline_status 215
set_fix_variable 112	set_title 215
set_font 209	set_true_manual_scaling 216
set_input_amounts 168	set_weight 33
set_interactive 8	setup file 9, 25, 29
set_interactive_mode 209, 242	show anchor 94, 201
set_label_curve_option 210	show grid 40, 88
set_log_file 242	show license information 38, 23

---

- 
- show triangular 88
  - show\_for\_t= 124
  - show\_value 172
  - simplified mode 74
  - Single-User-Node Locked-License (SUNLL) 6
  - site\_ratios 47
  - snap to grid 40
  - software development kit (SDK) 3
  - software updates 189
  - solution phase at fixed composition 177
  - special quantities 275
  - special quasi-random structures 53
  - species
    - keyword 8
  - species name 8
  - specify a parameter 121
  - spinodal curve 124
  - SQs 53
  - stability\_check 124
  - stable element reference 43
  - standalone computer 6
  - standalone installations 8, 20
  - start values 28
  - start\_simulation 233
  - start\_wizard 238
  - state variables 131, 190, 281, 288
  - status markers 40
  - step\_and\_map 124
  - step\_with\_options 137, 175
  - stepping calculation 151, 167
  - stepping operation 145
  - stoichiometric formula 9
  - stoichiometric phases 16
  - stop\_on\_error 244
  - store file 94, 108
  - store\_all\_weights 34
  - string command 25, 32
  - sublattice numbers 67
  - sublattices 15
  - submodules 119
  - subnet information 16
  - substitutional phase 11
  - substitutional solution phases 287
  - successor 28
  - successors 31, 48
  - suffixes 276
  - SUNLL 8
  - suspend\_phase\_in\_plot 216
  - suspended phase 134
  - switch axes 88
  - switch to console mode 33
  - switch to graphical mode 33
  - switch\_database 21, 252
-

---

symbols 190

    DATAPLOT 9, 30

symbolsize 22

syntax checker 37

SYS module 120

system definer 54, 59, 191

system requirements 3

systems of different orders 58

## T

t-zero\_temperature 124

T0 temperature simulation 151

TAB module 175

table

    keyword 32

table renderer 101, 199

table\_end 39, 19

table\_head 39, 19

table\_values 39, 19

tables

    DATAPLOT 7

tabulate 187, 216, 253

tabulate\_derivatives 254

tabulate\_reaction 258

tabulate\_substance 262

tabulating a reaction 176

tabulation of a substance 177

TC Aqueous Solution Database 163

---

TCAQ 163

TCBIN database 104

TDB file 32

temperature\_limits 16

temperature\_step 238

template 46

termination\_criteria 238

ternary calculator 106

ternary L parameter 65

ternary systems 21, 51, 37, 33

ternary\_diagram 268

ternary\_extrapolat 50

text command

    DATAPLOT 8

TGG Aqueous Solution Database 163

Thermo-Calc 16, 186, 7, 65

    databases 3

    installation 3

    macro file 25

Thermo-Calc Database Format (TDB) 3

Thermo-Calc software 3

thermodynamic

    database 3

    functions 175

    model parameters 13

    variables 270

thin client 6

---

---

thin client installations 31

tic\_type 16

tie lines 89

title command

    DATAPLOT 16

toggle\_alternate\_mode 124

toolbar 5, 32

tooltips 188

TP-functions 61, 64, 78, 82, 88, 95, 99, 102, 108

transfer\_start\_value 35

tree 28

triangular diagrams 37

troubleshooting installations 45

two-sublattice model 64

type-identifier 27

type\_definition 18

typical network client installations 27

typical standalone installations 21

typographical conventions 3

## U

u-fraction variable 276

u-fractions 135

unattended network client installation 35

uncertainty 24

uncertainty calculations 61, 64

uninstalling 57

---

updates

    manual or automatic 189

user databases 191

## V

version\_date 39

virtual coordinate system 5

## W

wild card characters 122

Windows installations 8

word coordinate system 5

work file 94

workspace files 126, 9, 29

## X

xlength 16

XQuartz 6, 17

xscale 15

xtext 15

xtype 15

## Y

ylength 16

yscale 15

ytext 15

ytype 16

## Z

zero phase fraction lines 141

---

Index: zero\_volume\_species – zoom in and out

---

zero\_volume\_species 43

zoom in and out 40