

POP files

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Calcul Thermodynamique

SATA / Giens Peninsula / 2017

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Introduction

- ▶ The thermodynamic assessment of a system provides a mathematical description of the Gibbs energy of all the phases of that system following three main steps:
 - ↪ the critical assessment of all the experimental and theoretical knowledge of the system,
 - ↪ the definition of models able to reproduce this knowledge,
 - ↪ the assessment of the parameters of the models.
- ▶ These three steps correspond roughly to the use of three modules of the Thermo-Calc package
 - ↪ EDIT_EXPERIMENTS,
 - ↪ GES,
 - ↪ PARROT.
- ▶ The present contribution focusses on the edition of the **POP** files defining the experimental values handled by the **EDIT_EXPERIMENTS** module.

What are POP files?

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- ▶ They are included in a `PAR` workspace where the optimisation will be run thanks to the `COMPILE_EXPERIMENTS` command of the `PARROT` module.

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- ▶ They are included in a `PAR` workspace where the optimisation will be run thanks to the `COMPILE_EXPERIMENTS` command of the `PARROT` module.
- ▶ The information they generate in the `PAR` workspace is generally modified during the optimisation procedure.

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- ▶ They are included in a `PAR` workspace where the optimisation will be run thanks to the `COMPILE_EXPERIMENTS` command of the `PARROT` module.
- ▶ The information they generate in the `PAR` workspace is generally modified during the optimisation procedure. It is worth keeping them updated because files generated automatically are not error-free and lose some comments and the table structure.

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It is the command EDIT_EXPERIMENTS that allows to go to this module from PARROT .
- ▶ Most of the commands available in this module are similar to the POLY_3 commands. They allow to define and compute an equilibrium.
- ▶ Specific commands are related to the optimisation procedure. They are used to
 - ↪ define and process many different equilibria,
 - ↪ define experimental values to fit and their uncertainty,
 - ↪ handle weights.

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- ▶ Specific commands are related to the optimisation procedure. They are used to
 - ↪ define and process many different equilibria,
 - ↪ define experimental values to fit and their uncertainty,
 - ↪ handle weights.

Some are not available in the interactive mode but only thanks to the use of POP files.

EDIT_EXPERIMENTS commands

ADVANCED_OPTIONS	GRAPHICS_PLOT	SELECT_EQUILIBRIUM
BACK	HELP	SET_ALL_START_VALUES
CHANGE_STATUS	IMPORT	SET_ALTERNATE_CONDITION
COMMENT	INFORMATION	SET_CONDITION
COMPUTE_ALL_EQUILIBRIA	LABEL_DATA	SET_NUMERICAL_LIMITS
COMPUTE_EQUILIBRIUM	LIST_ALL_EQUILIBRIA	SET_REFERENCE_STATE
CREATE_NEW_EQUILIBRIUM	LIST_CONDITIONS	SET_START_CONSTITUTION
DEFINE_COMPONENTS	LIST_EQUILIBRIUM	SET_START_VALUE
DELETE_SYMBOL	LIST_STATUS	SET_WEIGHT
ENTER_SYMBOL	LIST_SYMBOLS	SHOW_VALUE
EVALUATE_FUNCTIONS	MAKE_POP_FILE	STORE_ALL_WEIGHTS
EXIT	READ_WORKSPACES	TABLE_HEAD
EXPERIMENT	REINITIATE_MODULE	TRANSFER_START_VALUES
EXPORT	RESTORE_ALL_WEIGHTS	
FLUSH_BUFFER	SAVE_WORKSPACES	

EDIT_EXPERIMENTS commands

ADVANCED_OPTIONS

BACK

CHANGE_STATUS

COMMENT

COMPUTE_ALL_EQUILIBRIA

COMPUTE_EQUILIBRIUM

CREATE_NEW_EQUILIBRIUM

DEFINE_COMPONENTS

DELETE_SYMBOL

ENTER_SYMBOL

EVALUATE_FUNCTIONS

EXIT

EXPERIMENT

EXPORT

FLUSH_BUFFER

GRAPHICS_PLOT

HELP

IMPORT

INFORMATION

LABEL_DATA

LIST_ALL_EQUILIBRIA

LIST_CONDITIONS

LIST_EQUILIBRIUM

LIST_STATUS

LIST_SYMBOLS

MAKE_POP_FILE

READ_WORKSPACES

REINITIATE_MODULE

RESTORE_ALL_WEIGHTS

SAVE_WORKSPACES

SELECT_EQUILIBRIUM

SET_ALL_START_VALUES

SET_ALTERNATE_CONDITION

SET_CONDITION

SET_NUMERICAL_LIMITS

SET_REFERENCE_STATE

SET_START_CONSTITUTION

SET_START_VALUE

SET_WEIGHT

SHOW_VALUE

STORE_ALL_WEIGHTS

TABLE_HEAD

TRANSFER_START_VALUES

Commands available of all modules

EDIT_EXPERIMENTS commands

ADVANCED_OPTIONS

BACK

CHANGE_STATUS

COMMENT

COMPUTE_ALL_EQUILIBRIA

COMPUTE_EQUILIBRIUM

CREATE_NEW_EQUILIBRIUM

DEFINE_COMPONENTS

DELETE_SYMBOL

ENTER_SYMBOL

EVALUATE_FUNCTIONS

EXIT

EXPERIMENT

EXPORT

FLUSH_BUFFER

GRAPHICS_PLOT

HELP

IMPORT

INFORMATION

LABEL_DATA

LIST_ALL_EQUILIBRIA

LIST_CONDITIONS

LIST_EQUILIBRIUM

LIST_STATUS

LIST_SYMBOLS

MAKE_POP_FILE

READ_WORKSPACES

REINITIATE_MODULE

RESTORE_ALL_WEIGHTS

SAVE_WORKSPACES

SELECT_EQUILIBRIUM

SET_ALL_START_VALUES

SET_ALTERNATE_CONDITION

SET_CONDITION

SET_NUMERICAL_LIMITS

SET_REFERENCE_STATE

SET_START_CONSTITUTION

SET_START_VALUE

SET_WEIGHT

SHOW_VALUE

STORE_ALL_WEIGHTS

TABLE_HEAD

TRANSFER_START_VALUES

Commands identical to POLY_3 commands

EDIT_EXPERIMENTS commands

ADVANCED_OPTIONS

BACK

CHANGE_STATUS

COMMENT

COMPUTE_ALL_EQUILIBRIA

COMPUTE_EQUILIBRIUM

CREATE_NEW_EQUILIBRIUM

DEFINE_COMPONENTS

DELETE_SYMBOL

ENTER_SYMBOL

EVALUATE_FUNCTIONS

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GRAPHICS_PLOT

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IMPORT

INFORMATION

LABEL_DATA

LIST_ALL_EQUILIBRIA

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MAKE_POP_FILE

READ_WORKSPACES

REINITIATE_MODULE

RESTORE_ALL_WEIGHTS

SAVE_WORKSPACES

SELECT_EQUILIBRIUM

SET_ALL_START_VALUES

SET_ALTERNATE_CONDITION

SET_CONDITION

SET_NUMERICAL_LIMITS

SET_REFERENCE_STATE

SET_START_CONSTITUTION

SET_START_VALUE

SET_WEIGHT

SHOW_VALUE

STORE_ALL_WEIGHTS

TABLE_HEAD

TRANSFER_START_VALUES

Specific commands.

EDIT_EXPERIMENTS commands

ADVANCED_OPTIONS

BACK

CHANGE_STATUS

COMMENT

COMPUTE_ALL_EQUILIBRIA

COMPUTE_EQUILIBRIUM

CREATE_NEW_EQUILIBRIUM

DEFINE_COMPONENTS

DELETE_SYMBOL

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EVALUATE_FUNCTIONS

EXIT

EXPERIMENT

EXPORT

FLUSH_BUFFER

GRAPHICS_PLOT

HELP

IMPORT

INFORMATION

LABEL_DATA

LIST_ALL_EQUILIBRIA

LIST_CONDITIONS

LIST_EQUILIBRIUM

LIST_STATUS

LIST_SYMBOLS

MAKE_POP_FILE

READ_WORKSPACES

REINITIATE_MODULE

RESTORE_ALL_WEIGHTS

SAVE_WORKSPACES

SELECT_EQUILIBRIUM

SET_ALL_START_VALUES

SET_ALTERNATE_CONDITION

SET_CONDITION

SET_NUMERICAL_LIMITS

SET_REFERENCE_STATE

SET_START_CONSTITUTION

SET_START_VALUE

SET_WEIGHT

SHOW_VALUE

STORE_ALL_WEIGHTS

TABLE_HEAD

TRANSFER_START_VALUES

Specific commands mentioned in this lecture.

Singular equilibrium

```

$.....
$                                           Calo  1983 Sommer
$.....
CREATE_NEW_EQUILIBRIUM 350,1
CHANGE_STATUS PHASE LIQUID=ENT 1
SET_CONDITION P=PO N=1 T=1120 X(CU)=0.075
SET_REFERENCE_STATE CU LIQUID * 1E5
SET_REFERENCE_STATE MG LIQUID * 1E5
  EXPERIMENT HMR=-1900:5%
  LABEL AL
  COMMENT                               Liq - Calo - SOMMER
  GRAPHICS 5 .075 -1900 MS200

```

POLY_3 commands

```

$ .....
$                                           Calo  1983 Sommer
$ .....
CREATE_NEW_EQUILIBRIUM 350,1
CHANGE_STATUS PHASE LIQUID=ENT 1
SET_CONDITION P=PO N=1 T=1120 X(CU)=0.075
SET_REFERENCE_STATE CU LIQUID * 1E5
SET_REFERENCE_STATE MG LIQUID * 1E5
EXPERIMENT HMR=-1900:5%
LABEL AL
COMMENT                               Liq - Calo - SOMMER
GRAPHICS 5 .075 -1900 MS200

```

Usual POLY_3
commands

POP specific commands

```

$ .....
$                                           Calo  1983  Sommer
$ .....
CREATE_NEW_EQUILIBRIUM 350,1
CHANGE_STATUS PHASE LIQUID ENT 1
SET_CONDITION P=
SET_REFERENCE_ST
SET_REFERENCE_ST
EXPERIMENT HMR=
LABEL AL
COMMENT
GRAPHICS 5 .075

```

The definition of each equilibrium begins with the **CREATE_NEW_EQUILIBRIUM** command.

It requires a first integer corresponding to the identifier of the equilibrium. This identifier can be used in the **SELECT_EQUILIBRIUM** later on.

The second required integer is an initialisation code

↪ 0 : components and phases suspended

↪ 1 : components entered and phases suspended

↪ 2 : components and phases entered

POP specific commands

```

$ .....
$
$ .....
CREATE_NEW_EQUILIBRIUM 350,1
CHANGE_STATUS PHASE LIQUID=E
SET_CONDITION P=PO N=1 T=112
SET_REFERENCE_STATE CU LIQUID
SET_REFERENCE_STATE MG LIQUID
EXPERIMENT HMR=-1900:5%
LABEL AL
COMMENT
GRAPHICS 5 .075 -1900 MS200

```

The **EXPERIMENT** command defines the value of a quantity to be fitted as well as its uncertainty.

The uncertainty can be an absolute value or a relative percentage, as in this example.

Several **EXPERIMENT** commands can be given for an equilibrium, like the composition of several phases.

The **EXPERIMENT** command can be used with an inequality sign.

This command is optional. An equilibrium can be defined just to define a symbol.

POP specific commands

```

$ .....
$
$ .....
CREATE_NEW_EQUILIBRIUM
CHANGE_STATUS PHASE LI
SET_CONDITION P=PO N=1
SET_REFERENCE_STATE CU
SET_REFERENCE_STATE MG
EXPERIMENT HMR=-1900:
LABEL AL
COMMENT
GRAPHICS 5 .075 -1900

```

LABEL is an optional command. Its use is recommended to change easily the weight of all the equilibria having the same label.

The label is a string of maximum 4 characters, beginning with an A.

It is displayed - when selecting an equilibrium interactively, - on the first first line of the output of the **LIST_EQUILIBRIUM** and - in the second column of the output when giving the **COMPUTE_ALL_EQUILIBRIA**

Only one label is attached to an equilibrium. If several **LABEL** commands are given, the last one supersedes the previous ones.

This command can be given interactively.

It is forgotten in the POP files generated by the **MAKE_POP_FILE** command.

POP specific commands

```

$ .....
$ ..... Calo 1983 Sommer
$ .....
CREATE_NEW_EQUILIBRIUM 350,1
CHANGE_STATUS PHASE LIQUID=ENT 1
SET_CONDITION P=PO N=1 T=1120 X(CU)=0.075
SET_REFERENCE_STATE CU LIQUID * 1E5
SET_REFERENCE_STATE MG LIQUID * 1E5
EXPERIMENT HMR=-1900:5%
LABEL AL
COMMENT Liq - Calo - SOMMER
GRA

```

COMMENT is an optional command that cannot be given interactively. It defines a relatively short comment displayed - when giving LIST_EQUILIBRIUM before output options and - in the output of COMPUTE_ALL_EQUILIBRIA

MAKE_POP_FILE will introduce these comments in generated POP files.

POP specific commands

```

$ .....
$ ..... Calo 1983 Sommer
$ .....
CREATE_NEW_EQUILIBRIUM 350,1
CHANGE_STATUS PHASE LIQUID=E
SET_CONDITION P=PO N=1 T=112
SET_REFERENCE_STATE CU LIQUID * 1E5
SET_REFERENCE_STATE MG LIQUID * 1E5
EXPERIMENT HMR=-1900:5%
LABEL AL
COMMENT Liq - Calo - SOMMER
GRA

```

Longer comments are often introduced in the POP file on lines beginning by \$. These are not saved in the PAR workspace.

COMMENT is an optional command that cannot be given interactively. It defines a relatively short comment displayed - when giving LIST_EQUILIBRIUM before output options and - in the output of COMPUTE_ALL_EQUILIBRIA. MAKE_POP_FILE will introduce these comments in generated POP files.

POP specific commands

```

$ .....
$                                           Calo  1983 Sommer
$ .....
CREATE_NEW_EQUILIBRIUM 350,1
CHANGE_STATIC_PHASE LIQUID-ENT 1
SET_C
SET_L
SET_L
EXP PARROT module. The information is then not stored in the PAR
LABI workspace.
COMMENT                               Liq - Calo - SOMMER
GRAPHICS 5 .075 -1900 MS200

```

GRAPHICS is an optional command. It allows to define points in an exp file to be compared to calculated quantities. This file, named expfil.exp by default, is created when compiling the POP in the PARROT module. The information is then not stored in the PAR workspace.

POP specific commands

```
$ .....  
$                               Calo  1983  Sommer  
$ .....  
CREATE_NEW_EQUILIBRIUM 350,1  
CHANGE_STATUS_PHASE LIQUID-ENT 1  
SET_0  
SET_1  
SET_2  
EXPI PARROT module. The information is then not stored in the PAR  
LABI workspace.  
COMMENT                               Liq - Calo - SOMMER  
GRAPHICS 5 .075 -1900 MS200
```

GRAPHICS is an optional command. It allows to define points in an `exp` file to be compared to calculated quantities. This file, named `expfil.exp` by default, is created when compiling the POP in the PARROT module. The information is then not stored in the PARLABI workspace.

The integer just after the **GRAPHICS** command corresponds to the **DATASET** in the `exp` file. The next two numbers correspond to the coordinates of the point. The last item is the **GOC** (Graphical Operation Code).

Tables

- ▶ The definition of singular equilibria in `EDIT_EXPERIMENT` is, like in `POLY_3`, extremely flexible, allowing to compute any measured quantity.
- ▶ We have now introduced most of the specific commands of `EDIT_EXPERIMENTS` used in POP files:
 - ↪ `CREATE_NEW_EQUILIBRIUM`
 - ↪ `EXPERIMENTS`
 - ↪ `LABEL`
 - ↪ `COMMENT`
 - ↪ `GRAPHICS`
- ▶ Introducing single equilibria for many experiments is tedious. The use of tables is another power of `EDIT_EXPERIMENT`, only available in POP files.


```

TABLE_HEAD 300
CREATE_NEW_EQUILIBRIUM @@,1
CHANGE_STATUS PHASE CUMG2,LAVES=ENT 1
SET_CONDITION P=P0 N=1 x(Mg)=.5 T=@2
SET_REFERENCE_STATE MG HCP * 1E5
SET_ALL_START_VALUES F
EXPERIMENT MUR(MG)=@6:20%
COMMENT C15+CuMg2 - Mg PRESSURE - SMITH
GRAPHICS 4 @2 @6 MS2
LABEL @1
TABLE_VALUES
$      T/K  log p Mg (atm)  p Mg          a Mg          Mu Mg
AC2 675   -6.4800           3.3113E-07    0.0786        -14276
AC2 725   -5.6800           2.0893E-06    0.0839        -14937
AC2 775   -4.9832           1.0394E-05    0.0889        -15597
AC2 825   -4.3709           4.2569E-05    0.0935        -16258
AC2 875   -3.8286           1.4840E-04    0.0977        -16918
TABLE_END

```

TABLE_HEAD 300

```

CREATE_NEW_EQUILIBRIUM @@,1
CHANGE_STATUS PHASE CUMG2,LA
SET_CONDITION P=PO N=1 x(Mg)
SET_REFERENCE_STATE MG HCP *
SET_ALL_START_VALUES F
EXPERIMENT MUR(MG)=@6:20%
COMMENT C15+C
GRAPHICS 4 @2 @6 MS2
LABEL @1
TABLE_VALUES
$      T/K  log p Mg (atm)
AC2 675   -6.4800
AC2 725   -5.6800
AC2 775   -4.9832
AC2 825   -4.3709
AC2 875   -3.8286
TABLE_END

```

A table begins by **TABLE_HEAD** followed by an integer corresponding to the identifier of the first equilibrium of the table. The identifier of the equilibria will be automatically incremented by 1.

At the compilation of the POP file, individual equilibria are generated. The table structure is not stored in the PAR workspace. POP files written by MAKE_POP_FILE do not present any table.

TABLE_HEAD cannot be run interactively.

2.0893E-06	0.0839	-14937
1.0394E-05	0.0889	-15597
4.2569E-05	0.0935	-16258
1.4840E-04	0.0977	-16918

TABLE_HEAD 300

CREATE_NEW_EQUILIBRIUM @@,1

CHANGE_STATUS PHASE CUMG2,LA

SET_CONDITION P=P0 N=1 x(Mg)

SET_REFERENCE_STATE MG HCP *

SET_ALL_START_VALUES F

EXPERIMENT MUR(MG)=@6:20%

COMMENT

C15+CuMg2 - Mg PRESSURE - SMITH

GRAPHICS 4 @2 @6 MS2

LABEL @1

TABLE_VALUES

\$	T/K	log p Mg (atm)	p Mg	a Mg	Mu Mg
AC2	675	-6.4800	3.3113E-07	0.0786	-14276
AC2	725	-5.6800	2.0893E-06	0.0839	-14937
AC2	775	-4.9832	1.0394E-05	0.0889	-15597
AC2	825	-4.3709	4.2569E-05	0.0935	-16258
AC2	875	-3.8286	1.4840E-04	0.0977	-16918

TABLE_END

The identifier of the equilibrium being automatically generated, it is replaced by @@ in the CREATE_NEW_EQUILIBRIUM command.

```
TABLE_HEAD 300
CREATE_NEW_EQUILIBRIUM @@,1
CHANGE_STATUS PHASE CUMG2,LAVES=ENT 1
SET_CONDITION P=P0 N=1 x(Mg)=.5 T=@2
SET_REFERENCE_STATE MG HCP * 1E5
SET_ALL_START_VALUES F
```

@2 corresponds to
the content in the
second column.

```
EXPERIMENT MUR(MG)=@6:20%
COMMENT C15+CuMg2 - Mg PRESSURE - SMITH
GRAPHICS 4 @2 @6 MS2
LABEL @1
```

```
TABLE_VALUES
```

\$	T/K	log p Mg (atm)	p Mg	a Mg	Mu Mg
AC2	675	-6.4800	3.3113E-07	0.0786	-14276
AC2	725	-5.6800	2.0893E-06	0.0839	-14937
AC2	775	-4.9832	1.0394E-05	0.0889	-15597
AC2	825	-4.3709	4.2569E-05	0.0935	-16258
AC2	875	-3.8286	1.4840E-04	0.0977	-16918

```
TABLE_END
```

```
TABLE_HEAD 300
CREATE_NEW_EQUILIBRIUM @@,1
CHANGE_STATUS PHASE CUMG2,LAVES=ENT 1
SET_CONDITION P=P0 N=1 x(Mg)=.5 T=@2
SET_REFERENCE_STATE MG HCP * 1E5
SET_ALL_START_VALUES F
```

```
EXPERIMENT MUR(MG)=@6:20%
```

```
COMMENT C15+CuMg2 - Mg PRESSURE - SMITH
```

```
GRAPHICS 4 @2 @6 MS2
```

```
LABEL @1
```

```
TABLE_VALUES
```

\$	T/K	log p Mg (atm)	p Mg	a Mg	Mu Mg
AC2	675	-6.4800	3.3113E-07	0.0786	-14276
AC2	725	-5.6800	2.0893E-06	0.0839	-14937
AC2	775	-4.9832	1.0394E-05	0.0889	-15597
AC2	825	-4.3709	4.2569E-05	0.0935	-16258
AC2	875	-3.8286	1.4840E-04	0.0977	-16918

```
TABLE_END
```

@6 corresponds to
the content in the
sixth column.

```

TABLE_HEAD 300
CREATE_NEW_EQUILIBRIUM @@,1
CHANGE_STATUS PHASE CUMG2,LAVES=ENT 1
SET_CONDITION P=P0 N=1 x(Mg)=.5 T=@2
SET_REFERENCE_STATE MG HCP * 1E5
SET_ALL_START_VALUES F
EXPERIMENT MUR(MG)=@6:20%
COMMENT C15+CuMg2 - Mg PRESSURE - SMITH
GRAPHICS 4 @2 @6 MS2
LABEL @1
TABLE_VALUES
$      T/K  log p Mg (atm)
AC2 675  -6.4800
AC2 725  -5.6800
AC2 775  -4.9832
AC2 825  -4.3709
AC2 875  -3.8286
TABLE_END

```

@6 corresponds to the content in the sixth column.

@n can be used in any command of EDIT_EXPERIMENTS. Errors may appear at the compilation if its type doesn't respect the expectation of the command (integer, phase, string, ...)

```
TABLE_HEAD 300
CREATE_NEW_EQUILIBRIUM @@,1
CHANGE_STATUS PHASE CUMG2,LAVES=ENT 1
SET_CONDITION P=P0 N=1 x(Mg)=.5 T=@2
SET_REFERENCE_STATE MG HCP * 1E5
SET_ALL_START_VALUES F
EXPERIMENT MUR(MG)=@6:20
COMMENT C1
GRAPHICS 4 @2 @6 MS2
LABEL @1
```

TABLE_VALUES

\$	T/K	log p Mg (atm)	p Mg	a Mg	Mu Mg
AC2	675	-6.4800	3.3113E-07	0.0786	-14276
AC2	725	-5.6800	2.0893E-06	0.0839	-14937
AC2	775	-4.9832	1.0394E-05	0.0889	-15597
AC2	825	-4.3709	4.2569E-05	0.0935	-16258
AC2	875	-3.8286	1.4840E-04	0.0977	-16918

TABLE_END

The values of the table are introduced between **TABLE_VALUES** and **TABLE_END**.
 Columns are separated by at least one " ".
 Comments on the content of the columns are recommended.
 Some columns can be useless.

POLY_3 commands

- ▶ The definition of equilibria and experimental quantities to be fitted in `EDIT_EXPERIMENT` should be done as close as possible to the actual experiment.
 - ↪ The knowledge of the different variables defined by default in POLY-3 is key.
 - ↪ POLY_3 commands seldom used maybe needed in particular to define reference states and functions.
- ▶ The global minimisation is off by default in PAR workspaces and thus in `EDIT_EXPERIMENT`. It is recommended to keep it such. This requires a deeper knowledge of the commands handling starting values.

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- b(i): mass of i

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n=1 if #n not mentionned

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- **h**: enthalpy

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- $\mu(i)$: chemical potential of i
- $ac(i)$: activity of i

SET_REFERENCE_STATE

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Taking into account the new reference state is then possible adding `R` to the thermodynamic variables (`HMR`, `ACR(i)`, `MUR(i)`, ...)

Chemical potentials

```
CHANGE_STATUS PHASE FCC,LAVES=FIX 1
SET_CONDITION P=P0 T=751
SET_REFERENCE_STATE MG HCP * 1E5
SET_ALL_START_VALUES F
EXPERIMENT MUR(MG)=-30310:20%
```

*Note the use of * for the reference temperature.*

Mixing enthalpy in the liquid phase

```
CHANGE_STATUS PHASE LIQUID=ENT 1
SET_CONDITION P=P0 N=1 T=1100 X(Mg)=.075
SET_REFERENCE_STATE CU LIQUID * 1E5
SET_REFERENCE_STATE MG LIQUID * 1E5
EXPERIMENT HMR=-1900:5%
```

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SET_REFERENCE_STATE CU LIQUID * 1E5
SET_REFERENCE_STATE MG LIQUID * 1E5
EXPERIMENT HMR=-1900:5%
```

Using **HM** would have a different meaning. It would be the formation of the solution from the elements at room temperature. It can actually be the rough quantity measured. If it is given in the article, it is then better to fit this quantity rather than postprocessed value.

Formation energy of a compound

```
CHANGE_STATUS PHASE LAVES_C15=ENT 1
SET_CONDITION P=P0 T=298.15 N(Cu)=2 N(Mg)=1
SET_REFERENCE_STATE CU FCC_A1 * 1E5
SET_REFERENCE_STATE MG HCP_A3 * 1E5
EXPERIMENT HMR=-11171.3:420
```


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```

Note the way to define the ideal stoichiometry of a compound using $N(i)$ rather than $X(i)$.

Functions

Some thermodynamic properties require to be defined by the user, like the heat capacity, the heat increment, the melting enthalpy, the partial enthalpy, ...

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ENTER_SYMBOL FUNCTION CP=HM.T

HM.T is the derivative of the molar enthalpy versus T;
it is the heat capacity in J/mol/T if P is set as condition

ENTER_SYMBOL FUNCTION CPW=HW.T

HW.T is the heat capacity in J/g/T if P set as condition

ENTER_SYMBOL FUNCTION CPF=H.T

H.T is the heat capacity for the given number of component,
may be a compound formula if e.g. N(CU)=2, N(MG)=1

Partial enthalpy

```
@@ Partial entropy is  
ENTER_SYMBOL FUNCTION SMG=-MU(MG).T;  
@@ Partial enthalpy is  $h = g + s*t$   
ENTER_SYMBOL FUNCTION HMG=MU(MG)+SMG*T;
```

Enthalpy increment

Requires a reference equilibrium

```
CREATE_NEW_EQILIBRIUM 1,1  
CHANGE_STATUS PHASE LAVES_C15=ENTERED 1  
SET_CONDITION N(CU)=2 N(MG)=1 P=1E5 T=300  
ENTER_SYMBOL VARIABLE H300=H;
```

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CHANGE_STATUS PHASE LAVES_C15=ENTERED 1
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ENTER_SYMBOL VARIABLE H300=H;
```

And an equilibrium at the temperature
of the measurement

```
CREATE_NEW_EQUILIBRIUM 2,1
CHANGE_STATUS PHASE LAVES_C15=ENTERED 1
SET_CONDITION N(CU)=2 N(MG)=1 P=1E5 T=1000
ENTER_SYMBOL FUNCTION DHCU2MG=H-H300;
```

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CREATE_NEW_EQUILIBRIUM 1,1
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SET_CONDITION N(CU)=2 N(MG)=1 P=1E5 T=1000
ENTER_SYMBOL FUNCTION DHCU2MG=H-H300;
```

DHCU2MG can be used in EXPERIMENT command to compare with experimental enthalpy increment from reference temperature.

Melting enthalpy

Melting enthalpy also requires two equilibria when the melting is not congruent.

```
CREATE_NEW_EQUILIBRIUM 1,1
CHANGE_STATUS PHASE LAVES_C15=ENTERED 1
CHANGE_STATUS PHASE LIQUID=FIX 0
COMMENT SOLIDUS
SET_CONDITION N=1 X(CU)=.3 P=1E5
ENTER_SYMBOL VARIABLE HSOL=H;
```

```
CREATE_NEW_EQUILIBRIUM 2,1
CHANGE_STATUS PHASE LAVES_C15=ENTERED 1
CHANGE_STATUS PHASE LIQUID=FIX 1
COMMENT LIQUIDUS
SET_CONDITION N=1 X(CU)=.3 P=1E5
ENTER_SYMBOL FUNCTION HFUS=H-HSOL;
```

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In EDIT_EXPERIMENT, the phase status is for all phases by the CREATE_NEW_EQUILIBIRUM command.

- The codes 0 and 1 set all the phases suspended.
- The code 2 :set all phases entered.
- The status of a phase can then be changed to any of the 4 status with the usual CHANGE_STATUS command.

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```
CREATE_NEW_EQUILIBRIUM 1,1  
CHANGE_STATUS PHASE LAVES_C15=ENTERED 1  
CHANGE_STATUS PHASE LIQUID=FIX 0  
SET_CONDITION N=1 X(CU)=.3 P=1E5
```

This equilibrium corresponds to the solidus.

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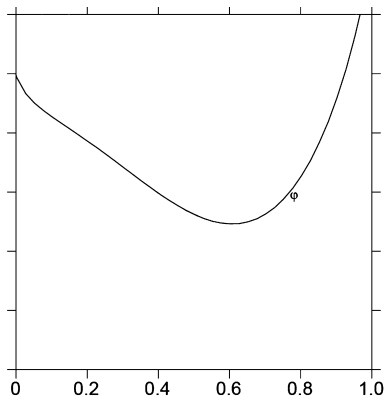
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Driving force

The driving force is one of the thermodynamic behaviour used in order to simulate the kinetic of phase precipitation. It has also some interest during a thermodynamic optimisation.

Driving force

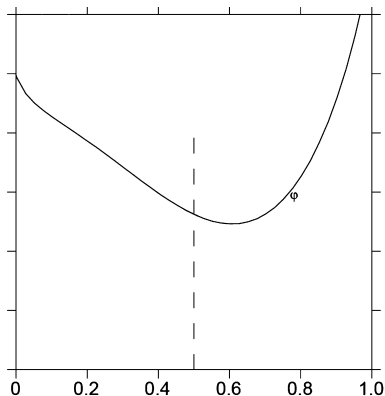
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Let's consider the single phase φ

Driving force

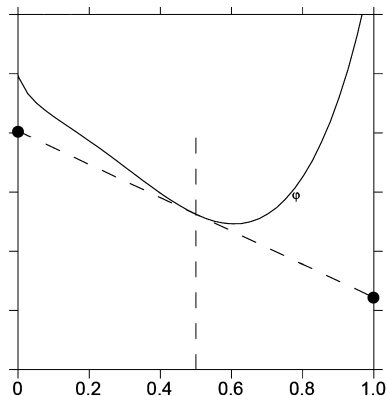
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Let's consider the single phase φ for $x_B=0.5$.

Driving force

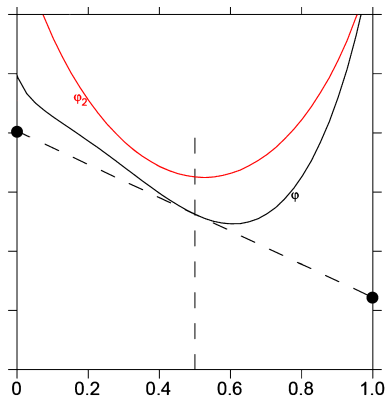
The driving force is one of the thermodynamic behaviour used in order to simulate the kinetic of phase precipitation. It has also some interest during a thermodynamic optimisation.



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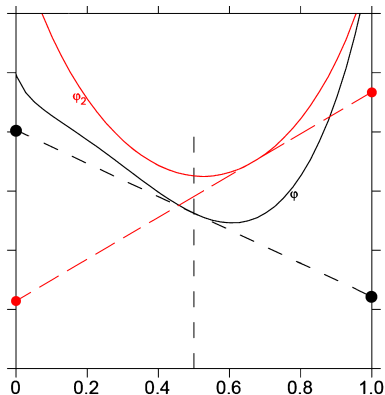


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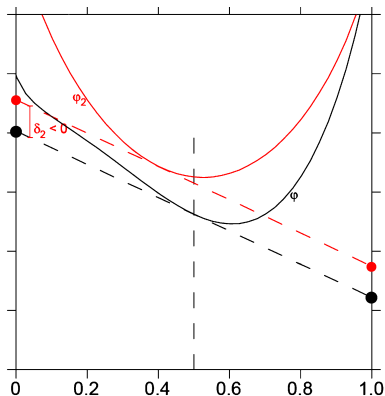


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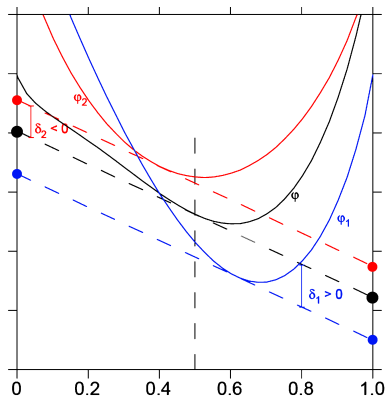


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The Gibbs energy of the phase φ_2 is above the one for the phase φ . For any composition, the tangent to φ_2 G curve defines chemical potentials for the elements. The difference between these potentials and the ones defined by the φ tangent is minimum where φ_2 tangent is parallel to φ tangent. The driving force of φ_2 corresponds to this minimum difference; it is negative in the present case.

Driving force

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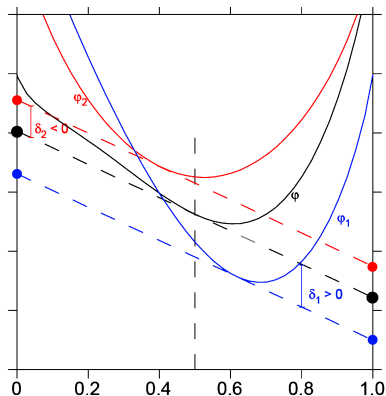


Let's consider the single phase φ for $x_B=0.5$. The tangent to the Gibbs energy at this point defines the chemical potentials of the elements where it intersects the axis corresponding to the pure elements.

The Gibbs energy curve of the phase φ_1 is below the one of the φ phase at the composition under consideration. The stable state at this composition is a two phase state $\varphi+\varphi_1$. The driving force of the φ_1 phase is positive, δ_1 . The point where the tangent to the φ_1 curve is parallel to the φ curve gives the composition of the first φ_1 phase precipitated in the φ phase of composition under consideration.

Driving force

The driving force is one of the thermodynamic behaviour used in order to simulate the kinetic of phase precipitation. It has also some interest during a thermodynamic optimisation.



Let's consider the single phase φ for $x_B=0.5$. The tangent to the Gibbs energy at this point defines the chemical potentials of the elements where it intersects the axis corresponding to the pure elements.

The Gibbs energy curve of the phase φ_1 is below the one of the φ phase at the composition under consideration. The stable state at this composition is a two phase state $\varphi+\varphi_1$. The driving force of the φ_1 phase is positive, δ_1 . The point where the tangent to the φ_1 curve is parallel to the φ curve gives the composition of the first φ_1 phase precipitated in the φ phase of composition under consideration.

The molar driving force of the phase alpha divided by RT is the variable $DGM(\alpha)$.

Starting values

As the global minimisation is turned off by default in PAR workspaces, computations fail more often. Some commands allow to start closer to the expected equilibrium and to converge more easily.

- ▶ `SET_START_VALUE` gives a starting value to a variable.
- ▶ `SET_START_CONSTITUTION` gives a starting constitution to a phase.

Starting values

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- ▶ `SET_START_CONSTITUTION` gives a starting constitution to a phase. After the phase name be given, a starting constitution can be entered in different formats.

Starting values

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- ▶ `SET_START_CONSTITUTION` gives a starting constitution to a phase.

```
SET_START_CONSTITUTION LIQUID NONE  
.99  
.01
```

after `NONE` or nothing, individual starting values are given for each constituent of the phase on each sublattice.

Starting values

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```
SET_START_CONSTITUTION LIQUID CU
```

Major constituent can be given on the line after phase name.

This does not work for setting major constituent in different sublattices.

Starting values

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- ▶ `SET_START_CONSTITUTION` gives a starting constitution to a phase.

```
SET_START_CONSTITUTION LIQUID *
```

* stands for a default constitution defined previously in GES with the `AMEND_PHASE_DATA` with option `MAJOR_CONSTITUTENT`.

Starting values

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- ▶ `SET_START_CONSTITUTION` gives a starting constitution to a phase.
- ▶ `SET_ALL_START_VALUES` gives a starting values to all variables.

Starting values

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`SET_ALL_START_VALUES` **N**/Y/F

N, default answer, requires to enter starting values, *i.e.* amount of entered phases (0 if N / 1 if Y) and amount of species in each sublattice, for each phase.

Starting values

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`SET_ALL_START_VALUES` N/Y/F

Y gives automatic starting values for each phase. The values correspond to a previous calculation, either for the current equilibrium or another one.

Starting values

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- ▶ `SET_START_CONSTITUTION` gives a starting constitution to a phase.
- ▶ `SET_ALL_START_VALUES` gives a starting values to all variables.

`SET_ALL_START_VALUES` N/Y/**F**

F gives an automatic value to all phase amounts and constitutions, forces to fresh starting values not related to previous results.

Starting values

As the global minimisation is turned off by default in PAR workspaces, computations fail more often. Some commands allow to start closer to the expected equilibrium and to converge more easily.

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- ▶ `SET_START_CONSTITUTION` gives a starting constitution to a phase.
- ▶ `SET_ALL_START_VALUES` gives a starting values to all variables.

`SET_ALL_START_VALUES N/Y/F`

Before Y/N/F, T or/and P are requested if they are not set as condition.

Starting values

As the global minimisation is turned off by default in PAR workspaces, computations fail more often. Some commands allow to start closer to the expected equilibrium and to converge more easily.

- ▶ `SET_START_VALUE` gives a starting value to a variable.
- ▶ `SET_START_CONSTITUTION` gives a starting constitution to a phase.
- ▶ `SET_ALL_START_VALUES` gives a starting values to all variables.

Extra tricks

```
CHANGE_STATUS PHASE FCC,LAVES=FIX 1
SET_CONDITION P=P0 T=751
SET_REFERENCE_STATE MG HCP * 1E5
SET_ALL_START_VALUES F
  EXPERIMENT MUR(MG)=-30310:20%
```

is identical to

```
CHANGE_STATUS PHASE FCC,LAVES=ENT 1
SET_CONDITION P=P0 T=751 X(Mg)=.2 N=1
SET_REFERENCE_STATE MG HCP * 1E5
SET_ALL_START_VALUES F
  EXPERIMENT MUR(MG)=-30310:20%
```

Extra tricks

```
CHANGE_STATUS PHASE FCC,LAVES=FIX 1
SET_CONDITION P=P0 T=751
SET_REFERENCE_STATE MG HCP * 1E5
SET_ALL_START_VALUES F
  EXPERIMENT MUR(MG)=-30310:20%
```

is identical to

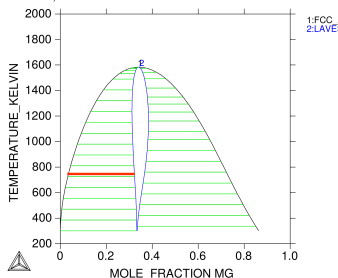
```
CHANGE_STATUS PHASE FCC,LAVES=ENT 1
SET_CONDITION P=P0 T=751 X(Mg)=.2 N=1
SET_REFERENCE_STATE MG HCP * 1E5
SET_ALL_START_VALUES F
  EXPERIMENT MUR(MG)=-30310:20%
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Extra tricks

```
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CHANGE_STATUS PHASE FCC,LAVES=ENT 1
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SET_ALL_START_VALUES F
  EXPERIMENT MUR(MG)=-30310:20%
```



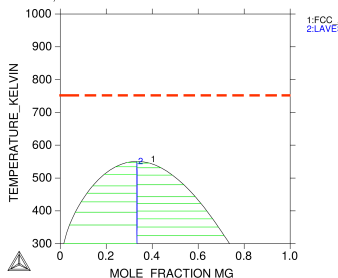
... when the phases are
in equilibrium at the
given temperature.

Extra tricks

```
CHANGE_STATUS PHASE FCC,LAVES=FIX 1
SET_CONDITION P=P0 T=751
SET_REFERENCE_STATE MG HCP * 1E5
SET_ALL_START_VALUES F
  EXPERIMENT MUR(MG)=-30310:20%
```

is identical to

```
CHANGE_STATUS PHASE FCC,LAVES=ENT 1
SET_CONDITION P=P0 T=751 X(Mg)=.2 N=1
SET_REFERENCE_STATE MG HCP * 1E5
SET_ALL_START_VALUES F
  EXPERIMENT MUR(MG)=-30310:20%
```



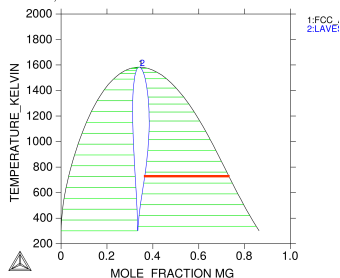
If not, the "fixed" equilibrium cannot be computed.

Extra tricks

```
CHANGE_STATUS PHASE FCC,LAVES=FIX 1
SET_CONDITION P=P0 T=751
SET_REFERENCE_STATE MG HCP * 1E5
SET_ALL_START_VALUES F
EXPERIMENT MUR(MG)=-30310:20%
```

is identical to

```
CHANGE_STATUS PHASE FCC,LAVES=ENT 1
SET_CONDITION P=P0 T=751 X(Mg)=.2 N=1
SET_REFERENCE_STATE MG HCP * 1E5
SET_ALL_START_VALUES F
EXPERIMENT MUR(MG)=-30310:20%
```



Moreover it can easily jump on the other side.

Extra tricks

```
CHANGE_STATUS PHASE FCC,LAVES=FIX 1
SET_CONDITION P=P0 T=751
SET_REFERENCE_STATE MG HCP * 1E5
SET_ALL_START_VALUES F
  EXPERIMENT MUR(MG)=-30310:20%
```

is identical to

```
CHANGE_STATUS PHASE FCC,LAVES=ENT 1
SET_CONDITION P=P0 T=751 X(Mg)=.2 N=1
SET_REFERENCE_STATE MG HCP * 1E5
SET_ALL_START_VALUES F
  EXPERIMENT MUR(MG)=-30310:20%
```

Setting composition
is better than
fixing phases.

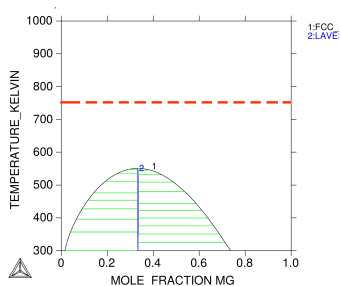
Driving force

When a phase does not appear where it should, the variable $DGM(ph)$ can be useful.

The use of this variable for every equilibrium is not recommended. It is usually introduced for few equilibria during the optimisation process to take into account qualitative information, if needed.

Driving force

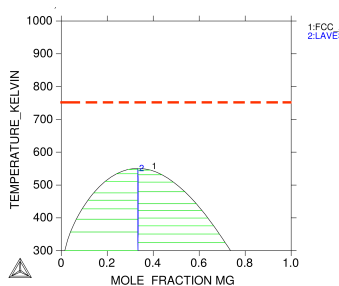
When a phase does not appear where it should, the variable $DGM(ph)$ can be useful.



Imagine that the LAVES phase should be stable at this temperature.

Driving force

When a phase does not appear where it should, the variable `DGM(ph)` can be useful.



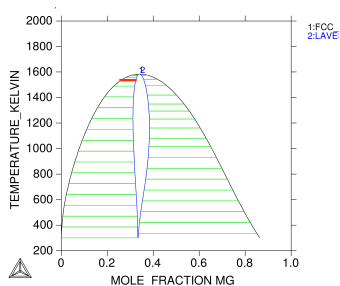
Imagine that the LAVES phase should be stable at this temperature.

EXPERIMENT `DGM(LAVES)=0:1e-7`

will help the LAVES phase to be stable at the given conditions.

Driving force

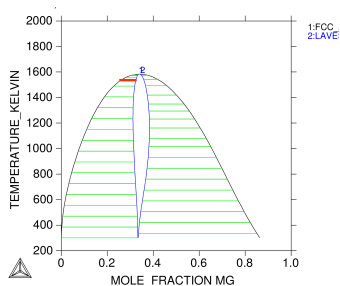
When a phase does not appear where it should, the variable $DGM(ph)$ can be useful.



Imagine that the LAVES phase should not be stable at this temperature.

Driving force

When a phase does not appear where it should, the variable $DGM(ph)$ can be useful.



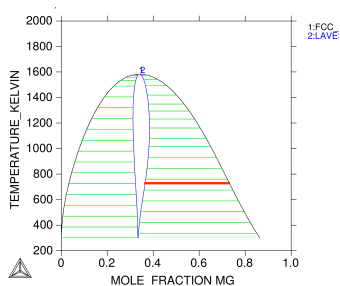
Imagine that the LAVES phase should not be stable at this temperature.

EXPERIMENT $DGM(LAVES) < -1e-5 : 1e-7$

will help the LAVES phase to be metastable at the given conditions.

Driving force

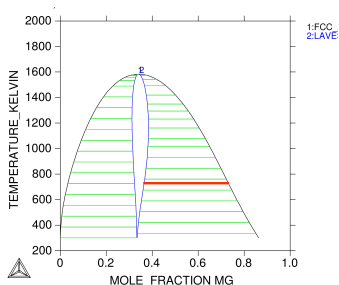
When a phase does not appear where it should, the variable $DGM(ph)$ can be useful.



Imagine that the CUMG2 phase should not be stable at this temperature.

Driving force

When a phase does not appear where it should, the variable $DGM(ph)$ can be useful.



Imagine that the CUMG2 phase should not be stable at this temperature.

```
CHANGE_STATUS PHASE CUMG2=DORMANT
EXPERIMENT DGM(CUMG2)>1e-5:1e-7
```

will help the CUMG2 phase to be more stable than the entered phases at the given conditions.

POP file

- ▶ You are now able to edit a POP file to run an optimisation.

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- ▶ It is not mandatory to introduce all the experimental available in a system in this file, in particular if some sets of data are disregarded for some reason or if the information is redundant.

POP file

- ▶ You are now able to edit a POP file to run an optimisation.
- ▶ It is not mandatory to introduce all the experimental available in a system in this file, in particular if some sets of data are disregarded for some reason or if the information is redundant.
- ▶ It is recommended comparing all experimental information with the computed values with the final description. This can be done using exp files (lecture of this afternoon).