POP files

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Calcul Thermodynamique

SATA / Toulouse / 2022

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Thermodynamic assessment

The thermodynamic assessment of a system provides a mathematical description of the Gibbs energy of all the phases of that system following 3 main steps:

1. critical assessment of all the experimental and theoretical knowledge of the system,
2. definition of models,
3. optimization of the model parameters in a least squares minimization.

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These 3 steps roughly correspond to the use of 3 advanced modules of the Thermo-Calc package

1. `EDIT-EXPERIMENTS`, now
2. `GES`, this afternoon
3. `PARROT`, tomorrow and later

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These 3 steps roughly correspond to the use of 3 advanced modules of the Thermo-Calc package

1. EDIT-EXPERIMENTS, now
2. GES, this afternoon
3. PARROT, tomorrow and later

This morning, we will learn how to write the POP files defining the equilibria handled by the module EDIT-EXPERIMENTS.

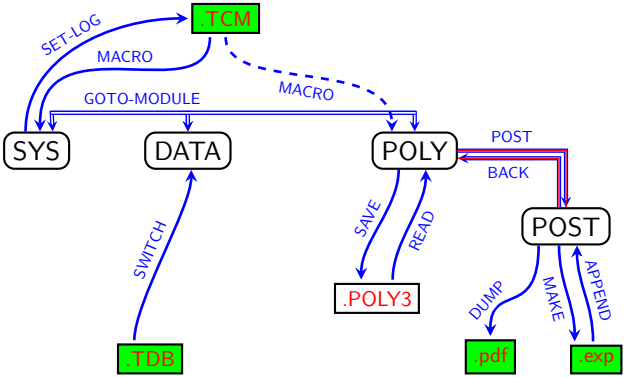
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What are POP files?

They are ASCII files defining the **conditions** of many equilibria corresponding to experimental states and **values measured** for that states. During the optimization, the difference between these values and the calculated ones will be minimised.

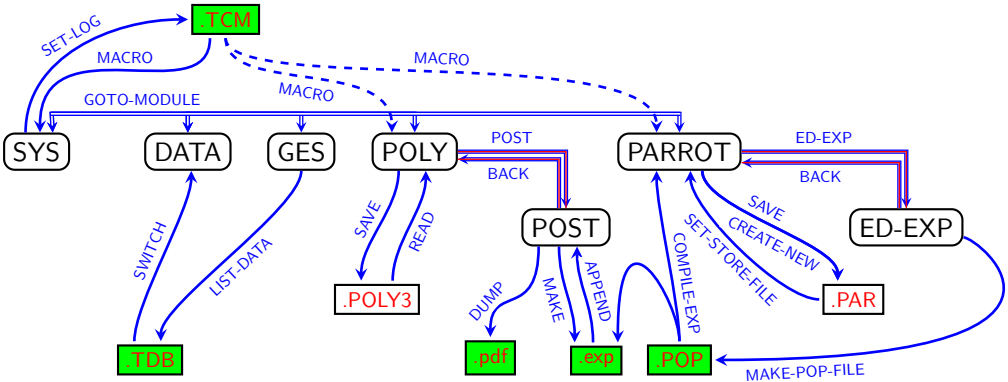
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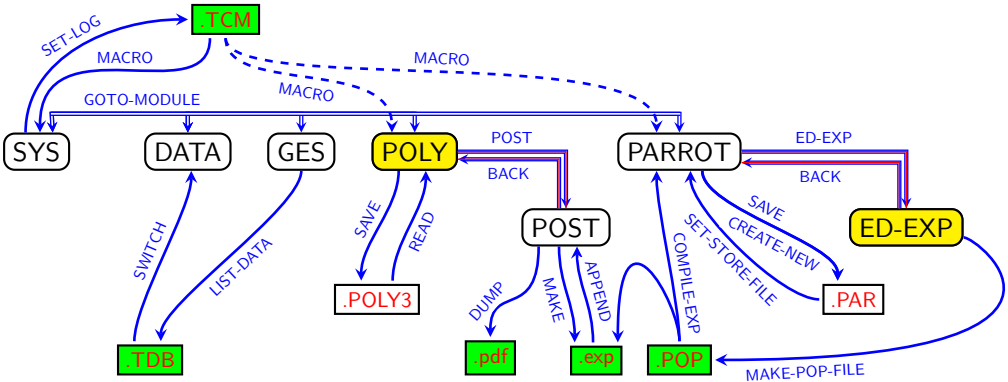
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EDIT-EXPERIMENTS commands

```
ADVANCED-OPTIONS          GRAPHICS-PLOT              RESTORE-ALL-WEIGHTS
BACK                      HELP                       SAVE-WORKSPACES
CHANGE-STATUS             IMPORT                     SELECT-EQUILIBRIUM
COMMENT                   INFORMATION                SET-ALL-START-VALUES
COMPUTE-ALL-EQUILIBRIA    LABEL-DATA                 SET-ALTERNATE-CONDITION
COMPUTE-EQUILIBRIUM       LIST-ALL-EQUILIBRIA        SET-CONDITION
CREATE-NEW-EQUILIBRIUM    LIST-CONDITIONS            SET-NUMERICAL-LIMITS
DEFINE-COMPONENTS         LIST-EQUILIBRIUM           SET-REFERENCE-STATE
DELETE-SYMBOL             LIST-STATUS                SET-START-CONSTITUTION
ENTER-SYMBOL              LIST-SYMBOLS               SET-START-VALUE
EVALUATE-FUNCTIONS        MAKE-COMPONENT-ENTERED     SET-WEIGHT
EXIT                      MAKE-COMPONENT-SUSPENDED   SHOW-VALUE
EXPERIMENT                MAKE-POP-FILE              STORE-ALL-WEIGHTS
EXPORT                    READ-WORKSPACES            TABLE-HEAD
FLUSH-BUFFER              REINITIATE-MODULE          TRANSFER-START-VALUES
```

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EDIT-EXPERIMENTS commands

General commands available in other modules

ADVANCED-OPTIONS	GRAPHICS-PLOT	RESTORE-ALL-WEIGHTS
BACK	HELP	SAVE-WORKSPACES
CHANGE-STATUS	IMPORT	SELECT-EQUILIBRIUM
COMMENT	INFORMATION	SET-ALL-START-VALUES
COMPUTE-ALL-EQUILIBRIA	LABEL-DATA	SET-ALTERNATE-CONDITION
COMPUTE-EQUILIBRIUM	LIST-ALL-EQUILIBRIA	SET-CONDITION
CREATE-NEW-EQUILIBRIUM	LIST-CONDITIONS	SET-NUMERICAL-LIMITS
DEFINE-COMPONENTS	LIST-EQUILIBRIUM	SET-REFERENCE-STATE
DELETE-SYMBOL	LIST-STATUS	SET-START-CONSTITUTION
ENTER-SYMBOL	LIST-SYMBOLS	SET-START-VALUE
EVALUATE-FUNCTIONS	MAKE-COMPONENT-ENTERED	SET-WEIGHT
EXIT	MAKE-COMPONENT-SUSPENDED	SHOW-VALUE
EXPERIMENT	MAKE-POP-FILE	STORE-ALL-WEIGHTS
EXPORT	READ-WORKSPACES	TABLE-HEAD
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EDIT-EXPERIMENTS commands

Commands identical to POLY-3 commands

ADVANCED-OPTIONS	GRAPHICS-PLOT	RESTORE-ALL-WEIGHTS
BACK	HELP	SAVE-WORKSPACES
CHANGE-STATUS	IMPORT	SELECT-EQUILIBRIUM
COMMENT	INFORMATION	SET-ALL-START-VALUES
COMPUTE-ALL-EQUILIBRIA	LABEL-DATA	SET-ALTERNATE-CONDITION
COMPUTE-EQUILIBRIUM	LIST-ALL-EQUILIBRIA	SET-CONDITION
CREATE-NEW-EQUILIBRIUM	LIST-CONDITIONS	SET-NUMERICAL-LIMITS
DEFINE-COMPONENTS	LIST-EQUILIBRIUM	SET-REFERENCE-STATE
DELETE-SYMBOL	LIST-STATUS	SET-START-CONSTITUTION
ENTER-SYMBOL	LIST-SYMBOLS	SET-START-VALUE
EVALUATE-FUNCTIONS	MAKE-COMPONENT-ENTERED	SET-WEIGHT
EXIT	MAKE-COMPONENT-SUSPENDED	SHOW-VALUE
EXPERIMENT	MAKE-POP-FILE	STORE-ALL-WEIGHTS
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EDIT-EXPERIMENTS commands

EDIT-EXPERIMENT Specific commands.

ADVANCED-OPTIONS	GRAPHICS-PLOT	RESTORE-ALL-WEIGHTS
BACK	HELP	SAVE-WORKSPACES
CHANGE-STATUS	IMPORT	SELECT-EQUILIBRIUM
COMMENT	INFORMATION	SET-ALL-START-VALUES
COMPUTE-ALL-EQUILIBRIA	LABEL-DATA	SET-ALTERNATE-CONDITION
COMPUTE-EQUILIBRIUM	LIST-ALL-EQUILIBRIA	SET-CONDITION
CREATE-NEW-EQUILIBRIUM	LIST-CONDITIONS	SET-NUMERICAL-LIMITS
DEFINE-COMPONENTS	LIST-EQUILIBRIUM	SET-REFERENCE-STATE
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ENTER-SYMBOL	LIST-SYMBOLS	SET-START-VALUE
EVALUATE-FUNCTIONS	MAKE-COMPONENT-ENTERED	SET-WEIGHT
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EXPERIMENT	MAKE-POP-FILE	STORE-ALL-WEIGHTS
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EDIT-EXPERIMENTS commands

Specific commands mentionned during this week.

ADVANCED-OPTIONS	GRAPHICS-PLOT	RESTORE-ALL-WEIGHTS
BACK	HELP	SAVE-WORKSPACES
CHANGE-STATUS	IMPORT	SELECT-EQUILIBRIUM
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COMPUTE-ALL-EQUILIBRIA	LABEL-DATA	SET-ALTERNATE-CONDITION
COMPUTE-EQUILIBRIUM	LIST-ALL-EQUILIBRIA	SET-CONDITION
CREATE-NEW-EQUILIBRIUM	LIST-CONDITIONS	SET-NUMERICAL-LIMITS
DEFINE-COMPONENTS	LIST-EQUILIBRIUM	SET-REFERENCE-STATE
DELETE-SYMBOL	LIST-STATUS	SET-START-CONSTITUTION
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EVALUATE-FUNCTIONS	MAKE-COMPONENT-ENTERED	SET-WEIGHT
EXIT	MAKE-COMPONENT-SUSPENDED	SHOW-VALUE
EXPERIMENT	MAKE-POP-FILE	STORE-ALL-WEIGHTS
EXPORT	READ-WORKSPACES	TABLE-HEAD
FLUSH-BUFFER	REINITIATE-MODULE	TRANSFER-START-VALUES

Single equilibrium

```
$.....................................................................
$                                                    Calo  1983 Sommer
$.....................................................................
CREATE-NEW-EQUILIBRIUM 350,1
CHANGE-STATUS PHASE LIQUID=ENT 1
SET-CONDITION P=P0 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

Usual POLY-3 commands

```
$.....................................................................
$                                                  Calo  1983 Sommer
$.....................................................................
CREATE-NEW-EQUILIBRIUM 350,1
CHANGE-STATUS PHASE LIQUID=ENT 1
SET-CONDITION P=P0 N=1 T=1120 X(CU)=0.075
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```

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POP specific commands

The definition of each single equilibrium begins with a CREATE-NEW-EQUILIBRIUM command.

```
$.....................................................................
$                                                    Calo  1983 Sommer
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CREATE-NEW-EQUILIBRIUM 350,1
CHANGE-STATUS PHASE LIQUID=ENT 1
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 COMMENT                              Liq - Calo - SOMMER
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```

It requires a first integer corresponding to the identifier of the equilibrium. This identifier can be used in the SELECT-EQUILIBRIUM command later on.

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 COMMENT                              Liq - Calo - SOMMER
 GRAPHICS 5 .075 -1900 MS200
```

The second required integer is an initialisation code

- 0 : components and phases suspended
- 1 : components entered and phases suspended
- 2 : components and phases entered

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

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

The uncertainty can be an absolute value or a relative percentage.

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

The uncertainty can be an absolute value or a relative percentage.

Several EXPERIMENT commands can be given for an equilibrium.

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

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Several EXPERIMENT commands can be given for an equilibrium.

The EXPERIMENT command can be used with an inequality sign.

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The use of LABEL allows afterwards to handle easily several equilibria with the SET-WEIGHT command.

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 LABEL AL
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 GRAPHICS 5 .075 -1900 MS200
```

The use of LABEL allows afterwards to handle easily several equilibria with the SET-WEIGHT command.

It requires a string begining by A of maximum 4 characters.

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The use of LABEL allows afterwards to handle easily several equilibria with the SET-WEIGHT command.

It requires a string begining by A of maximum 4 characters.

Only one label is attached to an equilibrium, the last one if several are given.

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 COMMENT                          Liq - Calo - SOMMER
 GRAPHICS 5 .075 -1900 MS200
```

The use of LABEL allows afterwards to handle easily several equilibria with the SET-WEIGHT command.

It requires a string begining by A of maximum 4 characters.

Only one label is attached to an equilibrium, the last one if several are given.

This command can be run interactively but it is not used by MAKE-POP-FILE.

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 LABEL AL
 COMMENT                          Liq - Calo - SOMMER
 GRAPHICS 5 .075 -1900 MS200
```

COMMENT is a command that cannot be given interactively.

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 COMMENT                              Liq - Calo - SOMMER
 GRAPHICS 5 .075 -1900 MS200
```

COMMENT is a command that cannot be given interactively.

MAKE-POP-FILE will introduce these short comments in POP files.

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 LABEL AL
 COMMENT                              Liq - Calo - SOMMER
 GRAPHICS 5 .075 -1900 MS200
```

COMMENT is a command that cannot be given interactively.

MAKE-POP-FILE will introduce these short comments in POP files.

They are short comments displayed
- when giving LIST-EQUILIBRIUM before output options and
- in the output of COMPUTE-ALL-EQUILIBRIA

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

```
$.....................................................................
$                                                  Calo  1983 Sommer
$.....................................................................
CREATE-NEW-EQUILIBRIUM 350,1
CHANGE-STATUS PHASE LIQUID=ENT 1
SET-CONDITION P=P0 N=1 T=1120 X(CU)=0.075
SET-REFERENCE-STATE CU LIQUID * 1E5
SET-REFERENCE-STATE MG LIQUID * 1E5
 EXPERIMENT HMR=-1900:5%
 LABEL AL
 COMMENT                              Liq - Calo - SOMMER
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$                                                    Calo  1983 Sommer
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CHANGE-STATUS PHASE LIQUID=ENT 1
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 EXPERIMENT HMR=-1900:5%
 LABEL AL
 COMMENT                          Liq - Calo - SOMMER
 GRAPHICS 5 .075 -1900 MS200
```

GRAPHICS allows to write points in an exp file to be compared to calculated quantities. This file is created when compiling the POP in the PARROT module. The information is then **not stored in the PAR workspace** and **not used by** MAKE-POP-FILE.

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).

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Tables

The definition of single equilibria in `EDIT-EXPERIMENT` is highly flexible, allowing to take into account any phase diagram or thermodynamic properties measured.

Introducing single equilibria for many experiments is tedious.

Tables, only available in `POP` files, are very usefull to handle experimental sets with many data.

Tables

A table begins by TABLE-HEAD followed by an integer corresponding to the identifier of the first equilibrium in the table.

```
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
```

The identifier of the following equilibria will be incremented by 1.
At the compilation of the POP file, single equilibria are created.
The table structure is **not stored** in the PAR workspace.
POP files written by MAKE-POP-FILE do not present any table.

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Tables

The identifier of the equilibrium being automatically generated, it is replaced by @@ in CREATE-NEW-EQUILIBRIUM.

```
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
```

Tables

@2 corresponds to the content in the second column under TABLE-VALUES.

```
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
```

Tables

@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)  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
```

Tables

@n can be used in any command of EDIT-EXPERIMENTS.

```
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
```

Tables

The values of the table are introduced between TABLE-VALUES and 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
```

Columns are separated by at least one space.
$Comments on the content of the columns are recommended.
Some columns can be useless.

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Advanced POLY-3 commands

The definition of the equilibria and of the measured properties to be fitted should be done as close as possible to the experiments.

This requires an advanced knowledge of the `POLY-3` commands.

- Starting values
- Variables
- Reference states
- Functions
- Driving force

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Starting values

As the global minimisation is turned off by default in PAR workspaces, computations fail more often than in usual calculations.

Some commands allow to start closer to the expected equilibrium and to converge more easily.

To give a starting value to one variable

```
SET-START-VALUE T=867
```

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Starting values

As the global minimisation is turned off by default in PAR workspaces, computations fail more often than in usual calculations.

Some commands allow to start closer to the expected equilibrium and to converge more easily.

To give a starting value to one variable

```
SET-START-VALUE T=867
```

To give a starting constitution to one phase

```
SET-START-CONSTITUTION FCC *
```

`*` stands for a default constitution defined previously in `GES` with the `AMEND-PHASE-DATA` with option `MAJOR-CONSTITUTENT`.

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Starting values

As the global minimisation is turned off by default in PAR workspaces, computations fail more often than in usual calculations.

Some commands allow to start closer to the expected equilibrium and to converge more easily.

To give a starting value to one variable

```
SET-START-VALUE T=867
```

To give a starting constitution to one phase

```
SET-START-CONSTITUTION FCC CU
```

Doesn't work when there are several sublattices

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Starting values

As the global minimisation is turned off by default in PAR workspaces, computations fail more often than in usual calculations.

Some commands allow to start closer to the expected equilibrium and to converge more easily.

To give a starting value to one variable

```
SET-START-VALUE T=867
```

To give a starting constitution to one phase

```
SET-START-CONSTITUTION FCC NONE
.99
.01
```

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Starting values

As the global minimisation is turned off by default in PAR workspaces, computations fail more often than in usual calculations.

Some commands allow to start closer to the expected equilibrium and to converge more easily.

To give a starting value to one variable

```
SET-START-VALUE T=867
```

To give a starting constitution to one phase

```
SET-START-CONSTITUTION LAVES NONE
.99
.01
.01
.99
```

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Starting values

As the global minimisation is turned off by default in PAR workspaces, computations fail more often than in usual calculations.

Some commands allow to start closer to the expected equilibrium and to converge more easily.

To give a starting value to one variable

```
SET-START-VALUE T=867
```

To give a starting constitution to one phase

```
SET-START-CONSTITUTION LAVES *
```

`*` stands for a default constitution defined previously in GES with the AMEND-PHASE-DATA with option MAJOR-CONSTITUTENT.

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Starting values

As the global minimisation is turned off by default in PAR workspaces, computations fail more often than in usual calculations.

Some commands allow to start closer to the expected equilibrium and to converge more easily.

To give a starting value to one variable

```
SET-START-VALUE T=867
```

To give a starting constitution to one phase

```
SET-START-CONSTITUTION LAVES *
```

`*` stands for a default constitution defined previously in GES with the `AMEND-PHASE-DATA` with option `MAJOR-CONSTITUTENT`.

To give starting values to all variables

```
SET-ALL-START-VALUES 867 N/Y/F
```

Before giving a code `N/Y/F`, a starting value for the temperature and the pressure should be given 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 than in usual calculations.

Some commands allow to start closer to the expected equilibrium and to converge more easily.

To give a starting value to one variable

```
SET-START-VALUE T=867
```

To give a starting constitution to one phase

```
SET-START-CONSTITUTION LAVES *
```

`*` stands for a default constitution defined previously in GES with the `AMEND-PHASE-DATA` with option `MAJOR-CONSTITUTENT`.

To give starting values to all variables

```
SET-ALL-START-VALUES 867 N
```

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

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As the global minimisation is turned off by default in PAR workspaces, computations fail more often than in usual calculations.

Some commands allow to start closer to the expected equilibrium and to converge more easily.

To give a starting value to one variable

```
SET-START-VALUE T=867
```

To give a starting constitution to one phase

```
SET-START-CONSTITUTION LAVES *
```

`*` stands for a default constitution defined previously in GES with the `AMEND-PHASE-DATA` with option `MAJOR-CONSTITUTENT`.

To give starting values to all variables

```
SET-ALL-START-VALUES 867 Y
```

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

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As the global minimisation is turned off by default in PAR workspaces, computations fail more often than in usual calculations.

Some commands allow to start closer to the expected equilibrium and to converge more easily.

To give a starting value to one variable

```
SET-START-VALUE T=867
```

To give a starting constitution to one phase

```
SET-START-CONSTITUTION LAVES *
```

`*` stands for a default constitution defined previously in GES with the `AMEND-PHASE-DATA` with option `MAJOR-CONSTITUTENT`.

To give starting values to all variables

```
SET-ALL-START-VALUES 867 F
```

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

Variables

Many variables are available in POLY-3 and thus in EDIT-EXPERIMENT.
They can be used as set condition or as experiment to fit.

T
temperature, in K

P
pressure, in Pa

n
number of mole

n(i)
number of mole of i

x(i)
atomic fraction of i

w(i)
mass fraction of i

x(alpha,i)
atomic fraction of i in the phase alpha

w(alpha,i)
mass fraction of i in the phase alpha

b(i)
mass of i, in g

np(alpha)
number of mole of the phase alpha

bp(alpha)
mass of alpha phase, in g

h
enthalpy, in J

h(alpha)
enthalpy of alpha phase, in J, 0 if np(alpha)=0

hm(alpha)
molar enthalpy of alpha phase, in J/mol, hm(alpha)= h(alpha)/np(alpha)

hw(alpha)
massic enthalpy of alpha phase, in J/g, hw(alpha)= h(alpha)/bp(alpha)

mu(i)
chemical potential of i

ac(i)
activity of i

y(alpha,i#n)
fraction of i in the sublattice n of the alpha phase, n=1 if #n not mentionned

dgm(alpha)
Driving force of the alpha phase, J/mol/RT

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Reference state

When considering experimental thermodynamic properties, it is key to use the proper reference state for the components.

By default the reference state for a component is SER : its stable state at 298.15K considered at 298.15K and 10^5Pa.

SET-REFERENCE-STATE i alpha Tvalue Pvalue

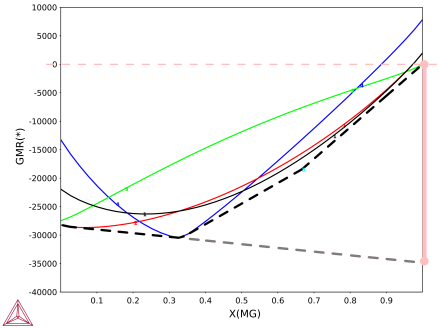
to define another reference state.
The phase `alpha` should be described for the pure component `i`.
Taking into account the new reference state is then possible adding `R` to the thermodynamic variables (`HMR`, `ACR(i)`, `MUR(i)`, ...)

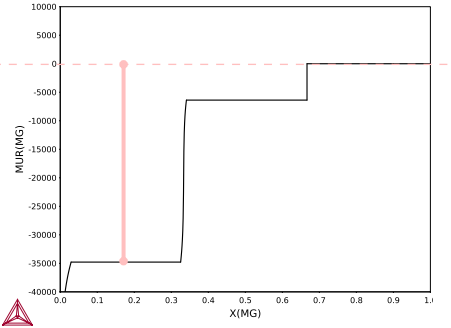
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Reference state - Chemical potentials

```
CHANGE-STATUS PHASE FCC,LAVES=FIX 1
SET-CONDITION P=P0 T=723
SET-REFERENCE-STATE MG HCP * 1E5
SET-ALL-START-VALUES F
 EXPERIMENT MUR(MG)=-34373:1050
```

* to use the current temperature for the reference state.



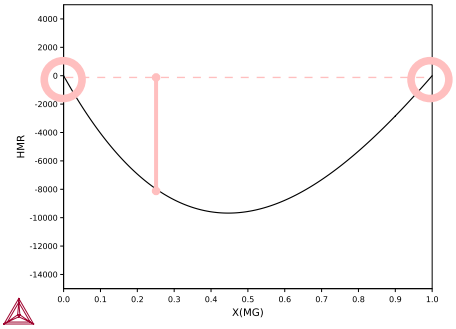


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Reference state - Mixing enthalpy in the liquid phase

```
CHANGE-STATUS PHASE LIQUID=ENT 1
SET-CONDITION P=P0 N=1 T=1100 X(Mg)=.25
SET-REFERENCE-STATE CU LIQUID * 1E5
SET-REFERENCE-STATE MG LIQUID * 1E5
 EXPERIMENT HMR=-8000:5%
```

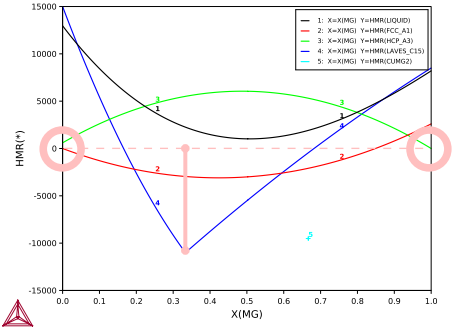
$(1-x)\ (\mathrm{Cu})_{liq} + x\ (\mathrm{Mg})_{liq} \rightarrow (\mathrm{Cu,Mg})_{liq}$



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Reference state - Formation enthalpy 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
```



$2\ (\mathrm{Cu})_{fcc} + (\mathrm{Mg})_{hcp} \rightarrow (\mathrm{Cu_2Mg})_{C15}$

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Functions

Some thermodynamic properties require to be defined by the user like:

- the heat capacity,
- the partial enthalpy,
- the heat increment,
- the melting enthalpy, ...

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Functions - Heat capacity

Cp in J/K/mol

```
ENTER-SYMBOL FUNCTION CP=HM.T;
```

Cp in J/K/g

```
ENTER-SYMBOL FUNCTION CPW=HW.T;
```

Cp in J/K/mol of formula

```
SET-CONDITION N(CU)=2 N(MG)=1
ENTER-SYMBOL FUNCTION CPF=H.T;
```

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Functions - Partial enthalpy

Partial entropy

```
ENTER-SYMBOL FUNCTION SMG=-MU(MG).T;
```

Partial enthalpy

```
ENTER-SYMBOL FUNCTION HMG=MU(MG)+SMG*T;
```

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Functions - Enthalpy increment

A reference equilibrium

```
CREATE-NEW-EQUILIBRIUM 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
```

And another one 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;
EXPERIMENT DHCU2MG=23752:1357
```

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Functions - Melting enthalpy

A reference equilibrium at the solidus

```
CREATE-NEW-EQUILIBRIUM 1,1
CHANGE-STATUS PHASE LAVES-C15=ENTERED 1
CHANGE-STATUS PHASE LIQUID=FIX 0
SET-CONDITION N=1 X(CU)=.32 P=1E5
ENTER-SYMBOL VARIABLE HSOL=H;
```

And another equilibrium at the liquidus

```
CREATE-NEW-EQUILIBRIUM 2,1
CHANGE-STATUS PHASE LAVES-C15=ENTERED 1
CHANGE-STATUS PHASE LIQUID=FIX 1
SET-CONDITION N=1 X(CU)=.32 P=1E5
ENTER-SYMBOL FUNCTION HFUS=H-HSOL;
EXPERIMENT HFUS=15200:1500
```

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Functions - Melting enthalpy

For congruent melting,
a single equilibrium can be used.

A reference equilibrium at the solidus

```
CREATE-NEW-EQUILIBRIUM 1,1
CHANGE-STATUS PHASE LAVES-C15=ENTERED 1
CHANGE-STATUS PHASE LIQUID=FIX 0
SET-CONDITION N=1 X(CU)=.32 P=1E5
ENTER-SYMBOL VARIABLE HSOL=H;
```

And another equilibrium at the liquidus

```
CREATE-NEW-EQUILIBRIUM 2,1
CHANGE-STATUS PHASE LAVES-C15=ENTERED 1
CHANGE-STATUS PHASE LIQUID=FIX 1
SET-CONDITION N=1 X(CU)=.32 P=1E5
ENTER-SYMBOL FUNCTION HFUS=H-HSOL;
EXPERIMENT HFUS=15200:1500
```

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Phase status

The status of the phases can be:

- ENTERED : default status in POLY-3,
- SUSPENDED : the phase is not considered during the calculations; however, it can be used as reference state for a constituent,
- FIXED : the phase must be present with the requested amount,
- DORMANT : the phase cannot appear but it is calculated, including its constitution so that its driving force is minimum.

In EDIT-EXPERIMENT, the phase status is initiated for all phases by the CREATE-NEW-EQUILIBRIUM 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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Phase status

The status of the phases can be:

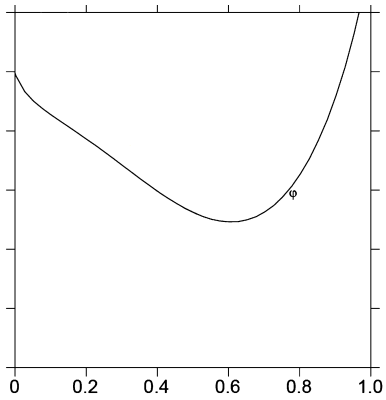
- ENTERED : default status in POLY-3,
- SUSPENDED : the phase is not considered during the calculations; however, it can be used as reference state for a constituent,
- FIXED : the phase must be present with the requested amount,
- DORMANT : the phase cannot appear but it is calculated, including its constitution so that its driving force is minimum.

In EDIT-EXPERIMENT, the phase status is initiated for all phases by the CREATE-NEW-EQUILIBRIUM 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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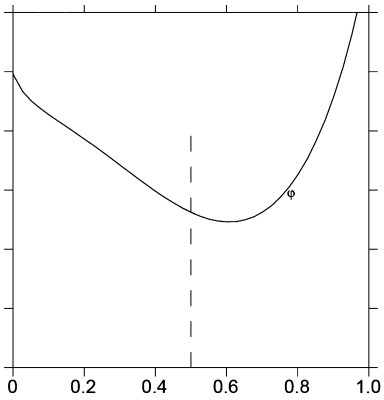
Driving force



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.

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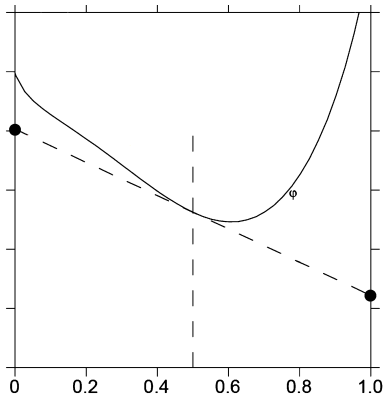
Driving force



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.

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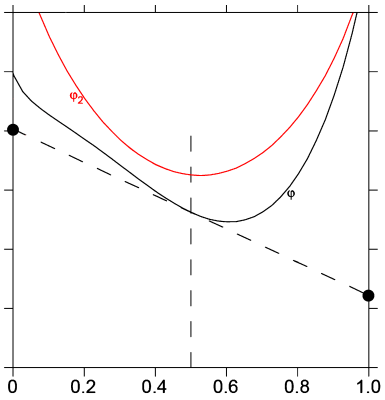
Driving force



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.

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Driving force

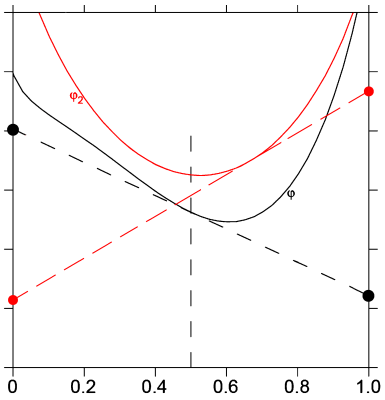


Let's consider the single phase φ for x_B=0.5. The tangent to the Gibbs energy at this point defines the chemical potentials of the elements where it intersects the axis corresponding to the pure elements.

The Gibbs energy 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 paralell to φ tangent. The driving force of φ_2 corresponds to this minimum difference; it is negative in the present case.

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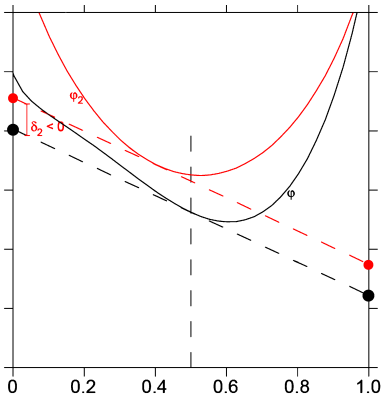


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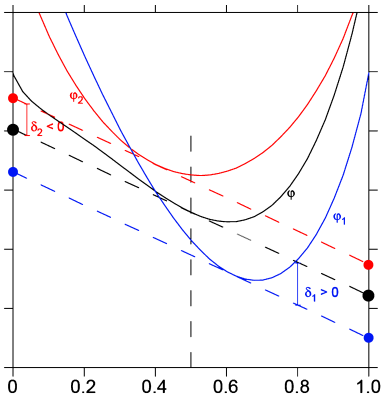


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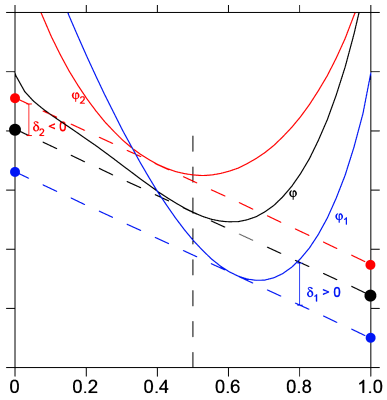


Let's consider the single phase φ for x_B=0.5. The tangent to the Gibbs energy at this point defines the chemical potentials of the elements where it intersects the axis corresponding to the pure elements.

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 φ+φ_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.

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

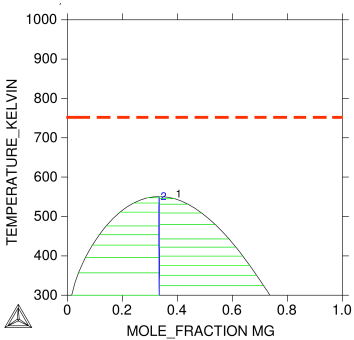
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Driving force

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

Driving force

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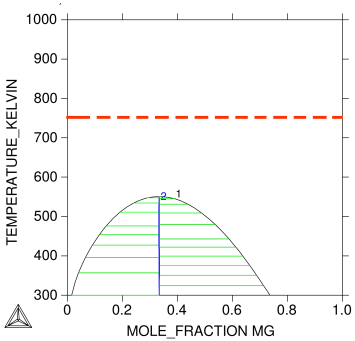


Imagine that the `LAVES` phase should be stable at this temperature.

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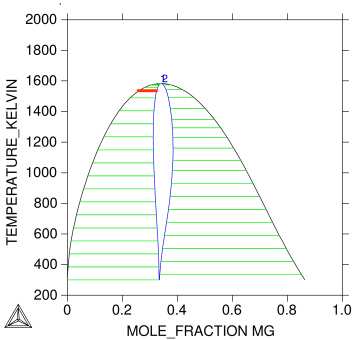
`EXPERIMENT DGM(LAVES)=0:1e-7`

will help the `LAVES` phase to be stable at the current conditions.

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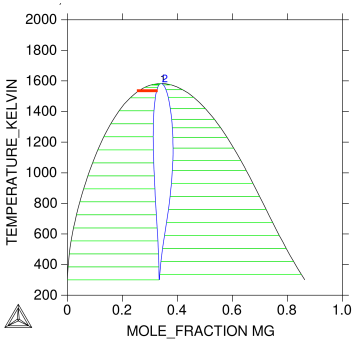
When a phase does not appear where it should, the variable `DGM(ph)` can be useful.



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

Driving force

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

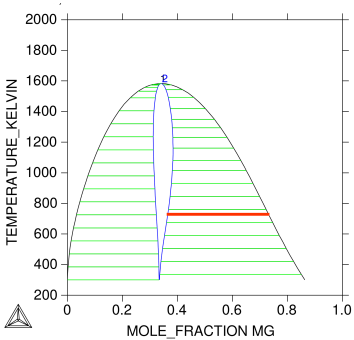
```
EXPERIMENT DGM(LAVES)<-1e-5:1e-7
```

will help the `LAVES` phase to be metastable at the current conditions.

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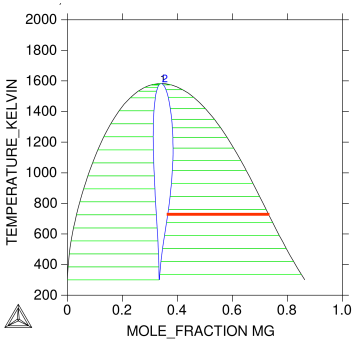
When a phase does not appear where it should, the variable `DGM(ph)` can be useful.



Imagine that the `CUMG2` 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 CUMG2 phase should be stable at this temperature.

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

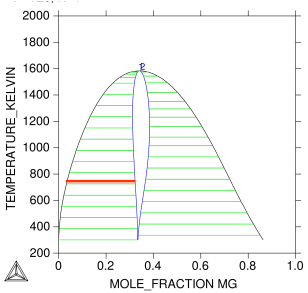
will help the CUMG2 phase to be more stable than the entered phases at the current conditions.

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Extra trick

```
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%
```

```
CHANGE-STATUS PHASE FCC,LAVES=ENT 1
SET-CONDITION P=P0 T=751
SET-CONDITION X(Mg)=.2 N=1
SET-REFERENCE-STATE MG HCP * 1E5
SET-ALL-START-VALUES F
 EXPERIMENT MUR(MG)=-30310:20%
```



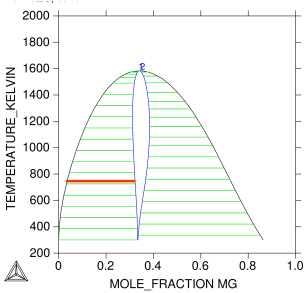
When everything goes well.

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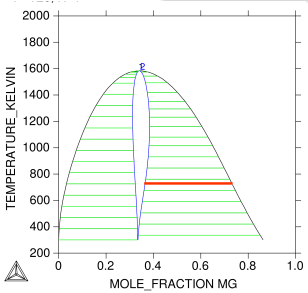
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SET-ALL-START-VALUES F
 EXPERIMENT MUR(MG)=-30310:20%
```



When everything goes well.

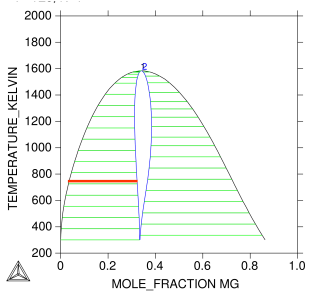


The calculated equilibrium is not the right one !

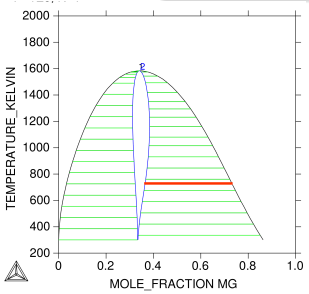
Extra trick

```
CHANGE-STATUS PHASE FCC,LAVES=FIX 1
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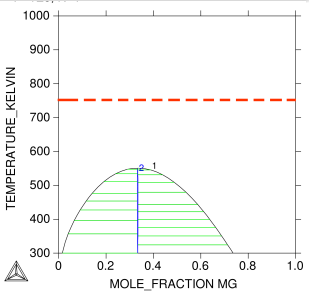
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```



When everything goes well.



The calculated equilibrium is not the right one !



The equilibrium cannot be calculated !

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POP file

You are now able to edit a `POP` file.

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

It is recommended to compare all experimental information with the computed values. This can be done using `exp` files (*this afternoon*).