exp and TCM files

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Calcul Thermodynamique

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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 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.

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

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

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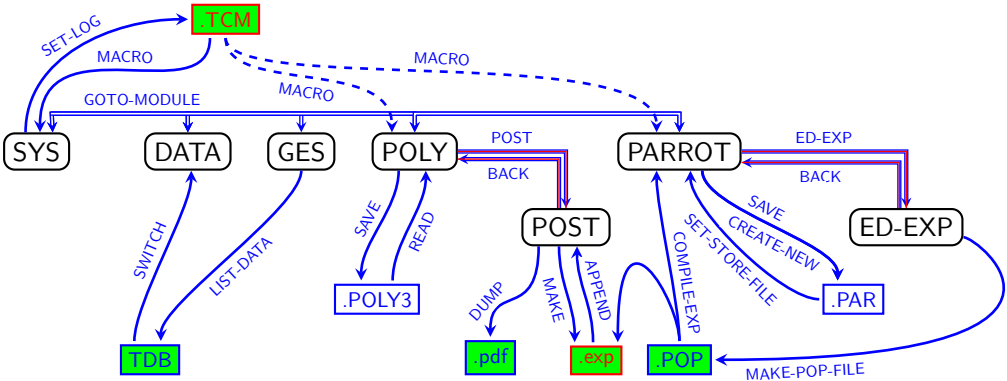
These 3 steps roughly correspond to the use of 3 advanced modules of the Thermo-Calc package

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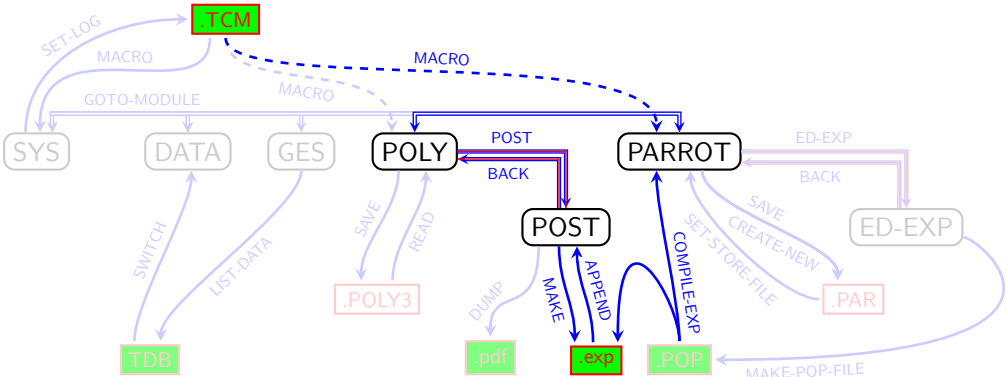
During the optimization, it is interesting to compare graphically calculated and experimental behaviors. This can be performed efficiently using

- `exp` files containing experimental data and
- `TCM` files containing commands running the calculations and the graphical comparison.

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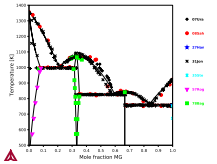
exp files - How are they used?

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in POST

APPEND-EXP

PLOT/DUMP



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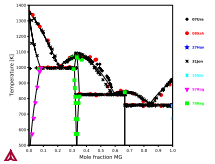
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PLOT/DUMP

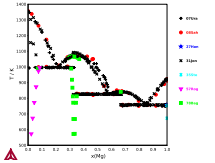


.exp

in POST

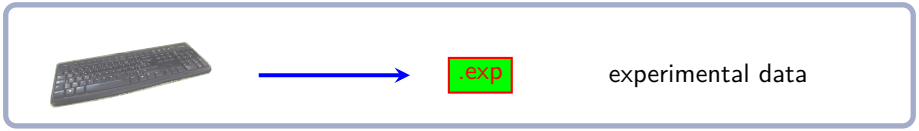
QUICK-EXP

PLOT/DUMP



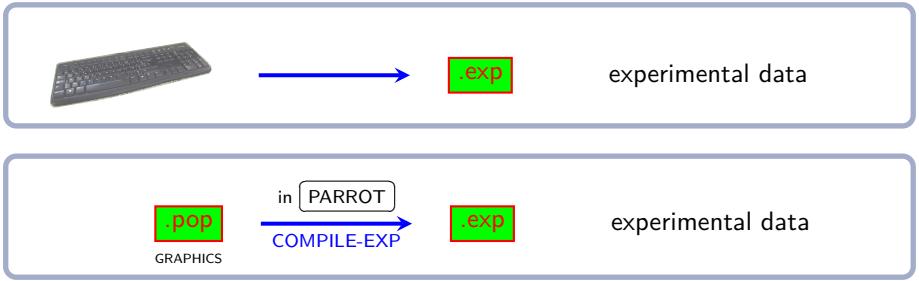
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.exp — experimental data

.pop (GRAPHICS) — in PARROT — COMPILE-EXP → .exp — experimental data

.POLY3 — in POST — MAKE-EXP → .exp — calculated data

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exp files structure

PROLOG

General information on the diagram:
axis scale, text, lenght, diagram type, title, ...

DATASET

Tables of points and how to treat them:
symbols, lines, colors, ...

```
PROLOG 1
   ---
   ---
   ---
PROLOG 2
   ---
   ---
   ---
PROLOG 3
   ---
   ---
   ---
DATASET 1
   ---
   ---
   ---
DATASET 2
   ---
   ---
   ---
DATASET 3
   ---
   ---
   ---
```

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PROLOG

```
PROLOG 1 Phase diagram
 XSCALE 0.0 1.0
 YSCALE 500 1400
 XTYPE LINEAR
 YTYPE LINEAR
 XLENGTH 11.5
 YLENGTH 11.5
 TITLE Cu-Mg
 XTEXT x(Mg)
 YTEXT T/K
```

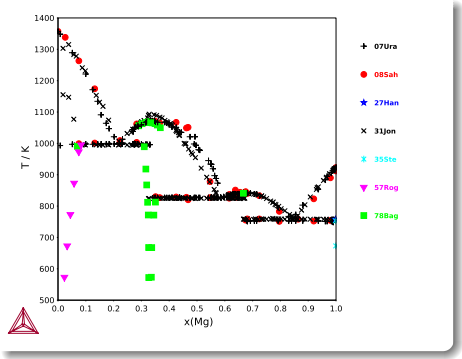
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```
DATASET 10 Phase diagram
ATTRIBUTE CENTER
CLIP OF
  color 2
  1.1 .8 MANS200' 08Sah
CLIP ON
BLOCK X=C1/100; Y=C2+273.15; GOC=C3,MAWS200
$ from table in original paper Sahmen
$ at% T/ degree C     liquidus
  0   1084
  2.6 1065
  7.5  990
 13.2  901
.....
BLOCKEND
```

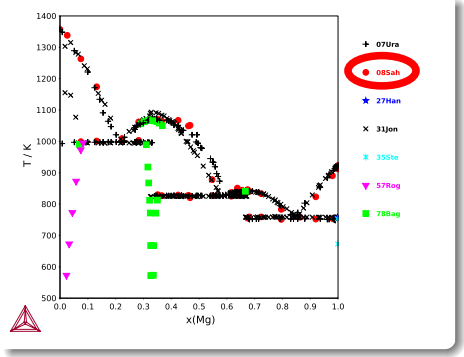
DATASET

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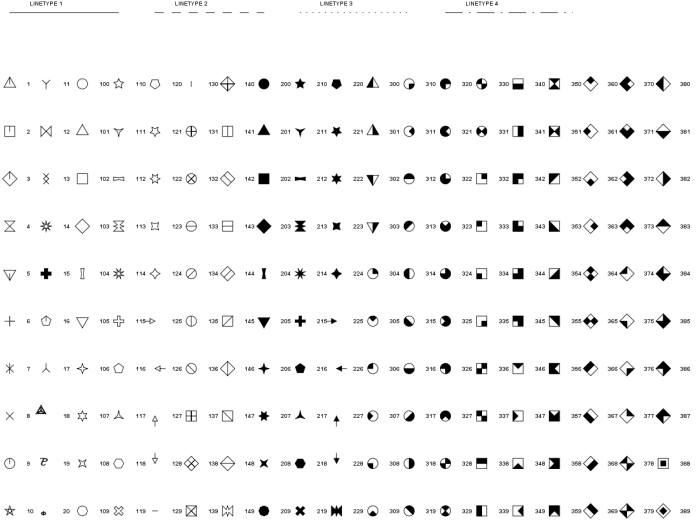


DATASET

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```

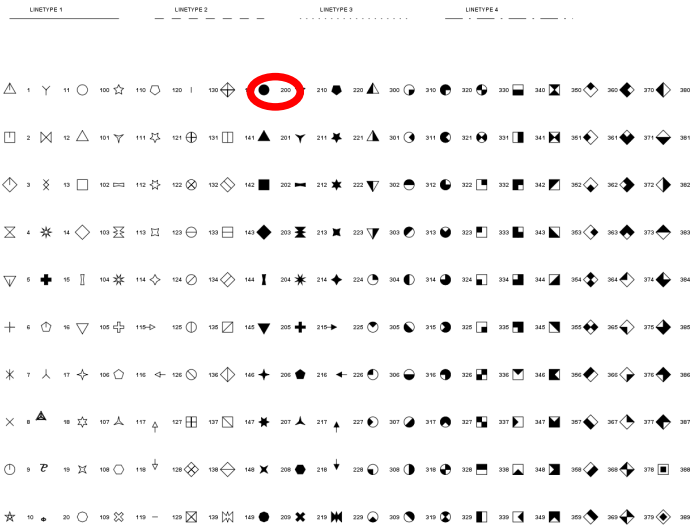


Symbols



To find this by yourself
F1 (Help/ Online Help)
Search for symbols

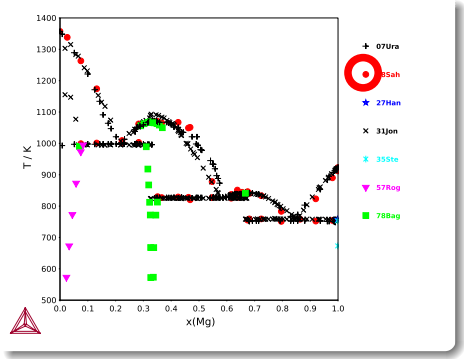
Symbols



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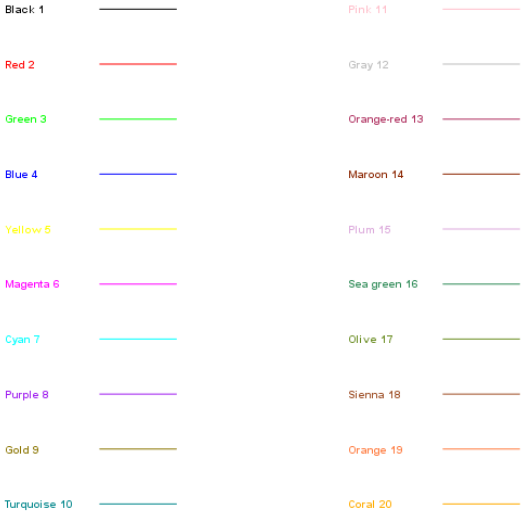
Symbols

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.....
BLOCKEND
```



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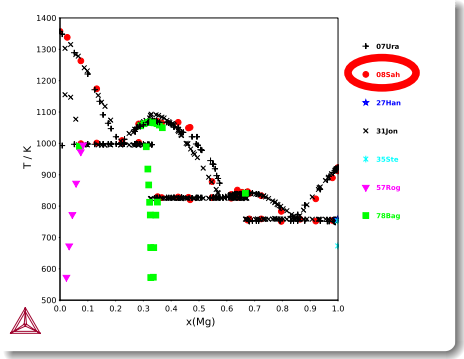
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Graphical Operation Code (GOC)

These are the available GOCs:

- `W`: World coordinates (* DEFAULT)
- `V`: Virtual coordinates
- `N`: Normalized plot box coordinates (NPC)
- `M`: Move to this XY (*)
- `D`: Draw to this XY
- `A`: XY is absolute values (*)
- `R`: XY are relative values
- `S`: Plot current symbol at XY
- `B`: Apply soft spines on the drawn curve (use only on BLOCK data)
- `S2`: Change current symbol to 2 and plot at XY
- `'`: Plot the following text at XY

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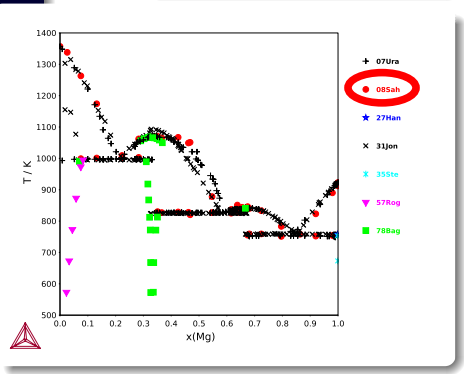
- W: World coordinates (* DEFAULT)
- V: Virtual coordinates
- N Normalized plot box coordinates (NPC)
- M Move to this XY (*)
- D: Draw to this XY
- A XY is absolute values (*)
- R: XY are relative values
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- S2 Change current symbol to 2 and plot at XY
- ' Plot the following text at XY

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Graphical Operation Code (GOC)

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ATTRIBUTE CENTER
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CLIP ON
BLOCK X=C1/100; Y=C2+273.15; GOC=C3,MAWS200
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$ at% T/ degree C      liquidus
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  2.6  1065
  7.5   990
 13.2   901
.....
BLOCKEND
```

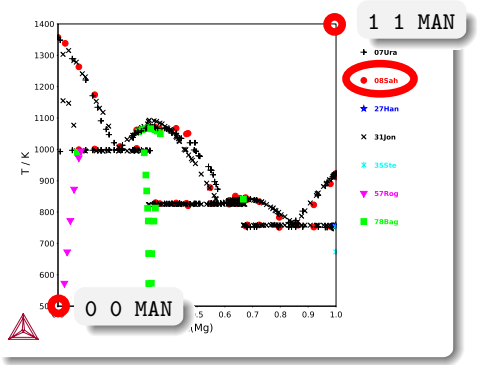
M Move to coordinates
A Absolute coordinates
N Normalized coordinates
' Add following string



Graphical Operation Code (GOC)

```
DATASET 10 Phase diagram
ATTRIBUTE CENTER
CLIP OF
  color 2
  1.1 .8 'MANS200' 08Sah
CLIP ON
BLOCK X=C1/100; Y=C2+273.15; GOC=C3,MAWS200
$ from table in original paper Sahmen
$ at% T/ degree C      liquidus
  0    1084
  2.6  1065
  7.5   990
 13.2   901
.....
BLOCKEND
```

M Move to coordinates
A Absolute coordinates
N Normalized coordinates
' Add following string

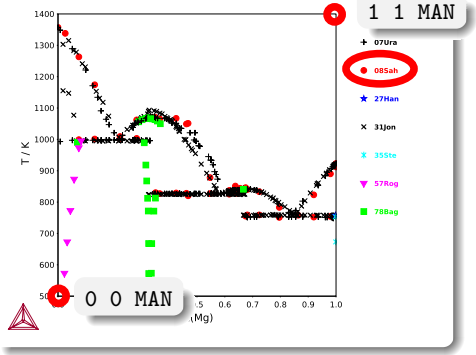


Graphical Operation Code (GOC)

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DATASET 10 Phase diagram
ATTRIBUTE CENTER
CLIP OF
  color 2
  1.1 .8 'MANS200' 08Sah
CLIP ON
BLOCK X=C1/100; Y=C2+273.15; GOC=C3,MAWS200
$ from table in original paper Sahmen
$ at% T/ degree C      liquidus
  0    1084
  2.6  1065
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 13.2   901
 .....
BLOCKEND
```

CLIP OF allows to write outside of the plotting box

M Move to coordinates
A Absolute coordinates
N Normalized coordinates
' Add following string



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```
BLOCK X=C1/100; Y=C2+273.15; GOC=C3,MAWS200
$ from table in original paper Sahmen
$ at% T/ degree C     liquidus
  0   1084
  2.6 1065
```

The points in this BLOCK are displayed

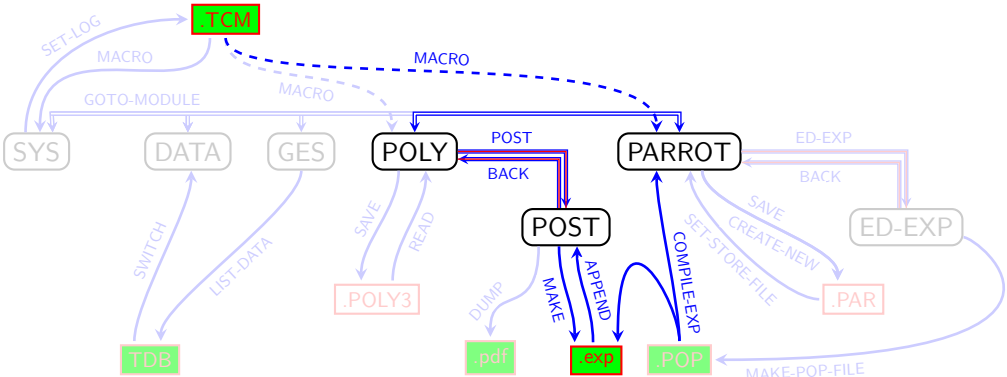
- . at x coordinate being the value in the 1st column (C1) divided by 100
- . at y coordinate being the value in the 2nd column (C2) +273.15
- . changes of the GOC for a point can be given in the 3rd column (C3)

but the default is

- . moving from a coordinate to the following (M) without drawing
- . at absolute coordinates (A)
- . in the world space (W)
- . as symbols (S), solid circle (200)

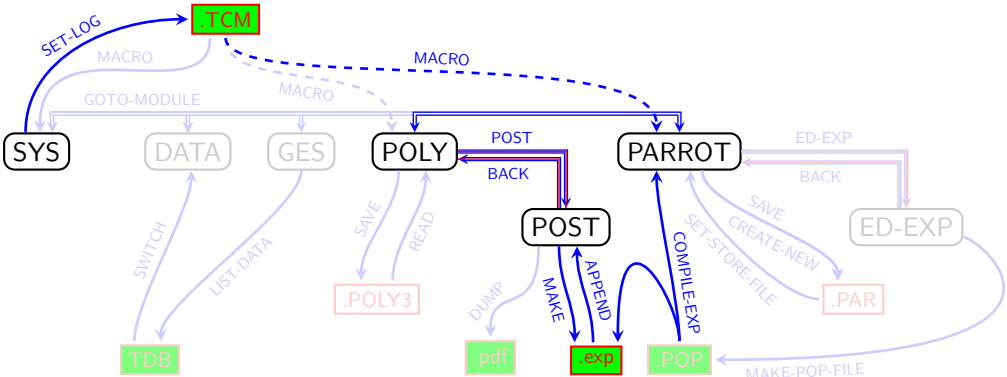
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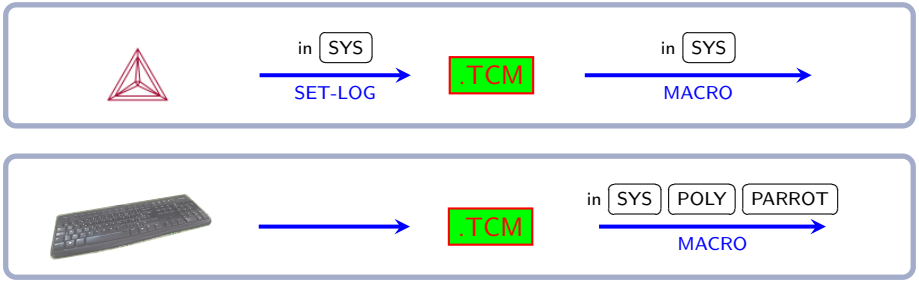
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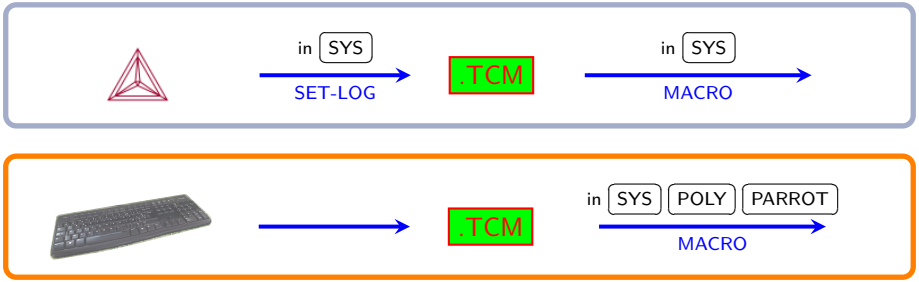
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SET-CONDITION
SET-REFERENCE-STATE
SET-AXIS-VARIABLE
SET-ALL-START-VALUES
MAP/STEP
POST
SET-DIAGRAM-AXIS
SET-AXIS-VARIABLE
APPEND-EXPERIMENTAL-DATA Y file 1:1
SELECT-PLOT
PLOT/DUMP
BACK
SET-INTERACTIVE
```

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DEFINE-COMPONENTS

In PAR workspaces, POLY-3 will get starting values (conditions, phase status, constituent fractions) from EDIT-EXPERIMENT.

In a TCM file to be used from PARROT, it is recommended to give systematically the command DEFINE-COMPONENTS to refresh the workspace. .

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DEFINE-COMPONENTS

In PAR workspaces, POLY-3 will get starting values (conditions, phase status, constituent fractions) from EDIT-EXPERIMENT.

In a TCM file to be used from PARROT, it is recommended to give systematically the command DEFINE-COMPONENTS to refresh the workspace. .

This command expects a list of components. By default, the new components will be the old ones. In addition to reinitiate all the values, it allows to define new components, for instance to use compounds rather than elements.

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Starting values

In PAR workspaces and embedded POLY, the **global minimisation is off**. It is recommended to keep it such to avoid the corruption of the PAR workspace.

This implies the need to give starting values to find the most stable state.

To give the starting constitution of 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 F
```

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

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APPEND-EXPERIMENTAL-DATA

APPEND-EXPERIMENTAL-DATA Y file.exp 1:1

This command allows to plot experimental points together with calculated results.
This command requests

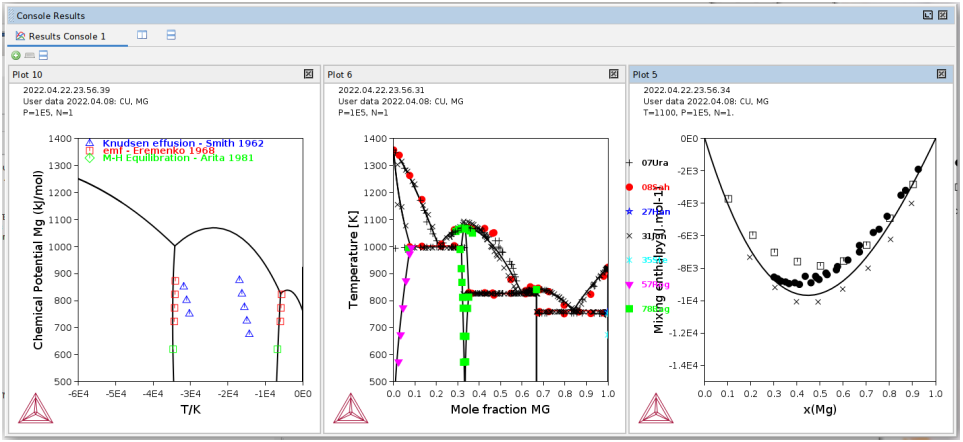
- Y/N to activate or deactivate the command, and if Y:
- an exp file name,
- one PROLOG number and if that number is not -1
- one or several DATASET number.

If the default PROLOG number -1 is given, the command displays the different DATASET short description appearing on the DATASET line in the exp file.

Several exp files can be considered if they are all given on the same line. PROLOG and DATASET numbers are then requested for each file. Only the last PROLOG is taken into account and all the DATASET.

SELECT-PLOT

allows to display the graphic in desired plot frame.
It makes easier to see the plot of different behaviours side by side.



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SET-INTERACTIVE

allows to continue interactively after the macro has been run.
This command has to be followed by an `EOL`.
Try to make that the macro ends in the same module where it starts.

Conclusion

You are now able to edit `exp` and `TCM` file in order to compare graphically calculated and experimental values during the course of an optimisation.