

exp and TCM files

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Calcul Thermodynamique

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- ▶ exp files
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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.
- ▶ It follows several steps:
 - the critical assessment of all the experimental and theoretical knowledge on the system under consideration,
 - the definition of models able to reproduce this knowledge,
 - the assessment of the parameters of the models.
- ▶ During the optimisation of the parameters, it is usual to compare the calculated behaviors with the corresponding experimental information. It is performed more efficiently using
 - **exp** files containing experimental data and
 - **TCM** files containing commands running the calculations and the graphical comparison.
- ▶ These files are in general also used in order to generate figures for the report of the assessment work.

What are exp files?

The exp files are used by the POST module in order to plot calculated and experimental points data.

How are they produced?

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 - generated at the compilation of a POP file following the information given by the command `GRAPHICS`,
 - edited by human being.
- ▶ The edition of automatically generated exp files is highly recommended in order to get nicer figures (colors, different type of symbols, labels).

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- ▶ The command `APPEND_EXPERIMENTAL_DATA` allows to represent the content of such a file together with results of calculations performed in the current `POLY_3` workspace.
- ▶ The commands `QUICK_EXPERIMENTAL_PLOT` allows to represent only the content of such a file.

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- ▶ The command `APPEND_EXPERIMENTAL_DATA` allows to represent the content of such a file together with results of calculations performed in the current `POLY_3` workspace.
- ▶ The commands `QUICK_EXPERIMENTAL_PLOT` allows to represent only the content of such a file.
- ▶ `PLOT_DIAGRAM` or `DUMP_DIAGRAM` commands are needed in order to take these commands into account in the graphical output.

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- ▶ The DATASET provides tables of points and how to treat them (symbols, lines, colors, ...)
- ▶ It can contain several PROLOG and several DATASET, identified by integers.

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
```

DATASET

```

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/C      liquidus
  0    1084
  2.6 1065
  7.5  990
 13.2  901
. . . . .
BLOCKEND

```

DATASET

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0 1084

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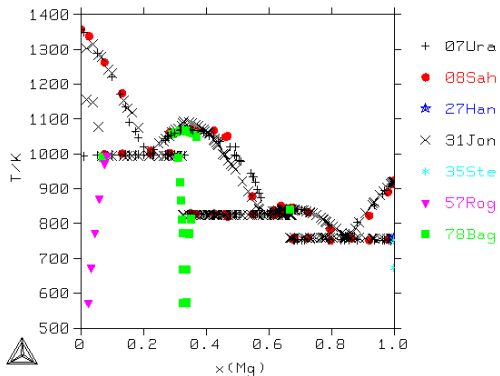
7.5 990

13.2 901

.....

BLOCKEND

THERMO-CALC (2015.06.15:02.05) : Cu-Mg



DATASET

The basic lines are constituted by X Y GOC
where GOC meaning Graphical Operating Code
is a combination of

- ↪ M move / D draw
- ↪ A absolute / R relative
- ↪ N normalized / W world
- ↪ S# symbol identified by integer #
- ↪ ' text

DATASET

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corresponds to

- ↪ a symbol (S), solid circle (200)
- ↪ at the absolute (A) coordinate 1.1 0.8
- ↪ normalized (N) to the axis
- ↪ followed by the text 08Sah

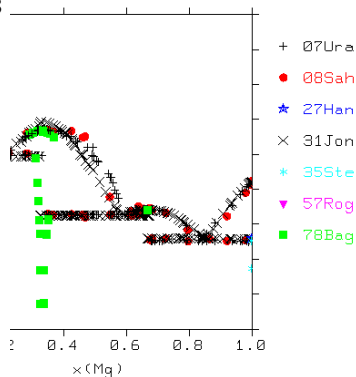
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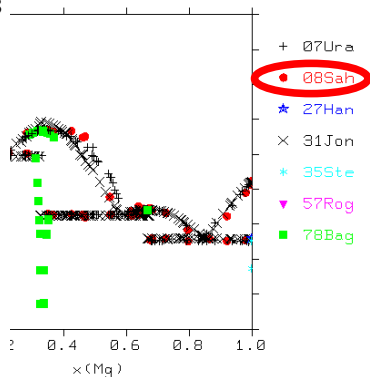
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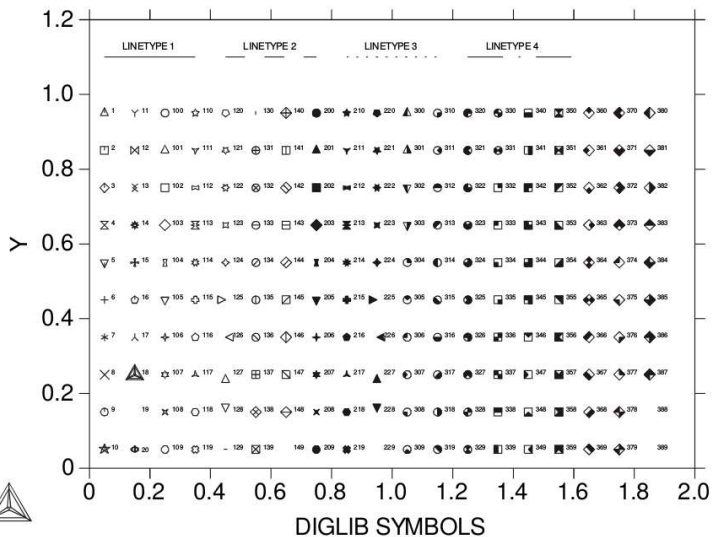
DATASET

A few more features of interest:

- \$ at the beginning of a line: comments
- CLIP OFF/ON enables to write out of the axis
- COLOR change of the color
- LINETYPE change of the line type
- SYMBOLSIZE change of the size of the symbols
- CHARSIZE change of the size of the texts
- ATTRIBUTE CENTER to center symbols/text

Symbols

THERMO-CALC (2001.08.21:15.04) : DIGLIB Symbols



Colors

Color Code: Color Effect

1: Black _____

2: Red _____

3: Green _____

4: Blue _____

5: Yellow _____

6: Magenta _____

7: Cyan _____

8: Purple _____

9: Gold _____

10: Turquoise _____

11: Pink _____

12: Gray _____

13: Orangered _____

14: Moroon _____

15: Plum _____

Color Code: Color Effect

16: Seagreen _____

17: Olivedrab _____

18: Sienna _____

19: Orange _____

20: Coral _____

21: UserDef _____

22 = 1 _____

23 = 1 _____

24 = 1 _____

25 = 1 _____

26 = 1 _____

27 = 1 _____

28 = 1 _____

29 = 1 _____

30 = 1 _____

BLOCK

Advanced operations can be applied to a set of points inside a BLOCK

```
BLOCK X=C1/100; Y=C2+273.15; GDC=C3,MAWS200
```

The points in that BLOCK are displayed

- ↪ as symbols (S), solid circle (200)
- ↪ at coordinates in the world space (W)
- ↪ x coordinate being the value in the 1st column (C1) divided by 100
- ↪ y coordinate being the value in the 2nd column (C2) +273.15
- ↪ changes of the GDC for a point are given in the 3rd column

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TCM files

The TCM files used during optimisation to compare experimental data to the description present some specific features. Commands of interest for such a file are listed hereunder.

```
GO POLY-3
DEFINE_COMPONENTS ...
SET_CONDITION ...
SET_REFERENCE_STATE ...
SET_AXIS_VARIABLE ...
SET_ALL_START_VALUES ...
MAP/STEP
POST
SET_DIAGRAM_AXIS ...
SET_AXIS_VARIABLE ...
APPEND_EXPERIMENTAL_DATAFILE Y file 1:1
PLOT/DUMP ...
SET_INTERACTIVE
```

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This command expects a list of component. By default, the new components will be the old ones.

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The following three commands can be used for that

- ▶ SET_START_VALUE
- ▶ SET_START_CONSTITUTION
- ▶ SET_ALL_START_VALUES

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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 will then be taken into account but all the DATASET indicated.