Tutorial of SUPCRTBL

Introductions to the files

supcrtBL.exe: the program for calculating the standard molal thermodynamic properties of minerals, gases, aqueous species, and reactions (Supcrt is an abbreviation for "supercritical").

dpronsbl.dat: The latest thermodynamic database compiled by students of Professor Zhu Chen at Indiana University – USA. The database includes thermodynamic properties for 225 minerals, 6 gas and 1406 aqueous species.

skarn.con: the file specifying reaction independent parameters such as the set of pressures and temperatures (this specific file gives you a table of answers at every 50 °C from 100 to 500°C, at pressure of 1000 bars. You can change the temperature and pressure to whatever values you are interested in).

example.rxn: the reaction file specifies the following three reactions

1. $Na^+ + Cl^- = NaCl(aq)$
2. $CO_2(g) + H_2O = HCO_3^- + H^+$
3. $Albite + 4H^+ = Na^+ + Al^{3+} + 3SiO_2(aq) + 2H_2O$

How to use SUPCRTBL to calculate the equilibrium constants

The program is interactive, with a number of options at each step. The following instructions are sufficient to get you started and to do the problem sets, but do not compass all possibilities. If you get lost, hit Ctrl+C, and start again.

Make sure supcrtBL.exe, dpronsbl.dat, skarn.con, and example.rxn are in the same folder.

Steps:

(1) Double click supcrtBL.exe.

(2) *Would you like to use the default thermodynamic database?*

Y *(if you want to use database other than dpronsbl.dat, type N and then type in the name of the database)*

(3) *Choose file option for specifying reaction-independent parameters.*

1= select one of three default files.

2= select an existing non-default files.

3= build a new file.

SUPCRT wants to know what values of T and P you need answers for. The three options under no. 1 are often sufficient, and if so, type "1" and hit ENTER. If you want a range of T and P not included in the choices under 1 (for example 20 to 1000 °C at 1 bar), type "3" or select a non-default file built in advance.

Here we select 2.

(4) *Specify the file name:*

skarn.con

(5) *Choose file option for specifying reactions. You have the choice of 1 and 2.*

1= using an existing reaction files.

2= build a new reaction file.

You must now specify the reaction you are interested in. If you have done this before, and saved it in a file, choose "1", and then give the file name when prompted. If this is something new, type "2", and hit ENTER.

Since we already have the reaction file, we can just type "1" here. However, if you want to build a new reaction file, you can choose "2" and proceed to step (9).

(6) *specify name of reaction file:*

example.rxn

(7) *specify name for tabulated output file:*

Output.txt (You can pick any name you like.)

(8) *Specify option for X-Y plot files. You have three choices.*

In generally we choose 1.

reaction in progress. . .
. . . a few more messages. . .
. . . execution completed
Your results should now be in the file with the name you specified.

If you choose "2" at step (5), please follow step (9) – step (16).

Take the reaction

$NaAlSi_3O_8$ (Albite) + $4H^+$ = Al^{3+} + Na^+ + $3SiO_2$(aq) + $2H_2O$

for example.

(9) *Specify the number of reactions:*

1 (in this case)

(10) *Title of reaction:*

Albite (in this case)

(11) *enter [coe_ species] pairs, separated by blanks, one pair per line, for reaction 1 (conclude with [0 done]). (note: in the left of the equation use negative sign and in the right use positive sign and this program is CASE SENSITIVE)*

-1 ALBITE

-4 H+

1 Al+3

1 Na+

3 SiO2,aq (don't forget the "aq")

2 H2O

0

(12) *reaction 1 stoichiometry. Is this correct?*

If you made an error, type "n", and repeat. Otherwise type "Y".

(13) *Do you want to save?*

Y

(14) *Name:*

Albite (Next time you can use this reaction file to save the time of preparing input file. from step (5). Choose 1.)

(15) *Name out put file:*

albite.txt

(16) *Generate X-Y plot?*

1

Reference:

Johnson J.W., Oelkers E. H. and Helgeson H. C. (1992), SUPCRT92: a software package for calculating the standard molal thermodynamic properties of minerals, gases, aqueous species, and reactions from 1 to 5000 bar and 0 to 1000°C, *Computers & Geosciences Vol. 18, No. 7, pp. 899-947, 1992*.

Zimmer K., Zhang Y., Peng L., Zhang G., and Zhu C. (2015), SUPCRTBL: A revised and extended thermodynamic dataset and software package of SUPCRT92, manuscript submitted to *Computers & Geosciences*