Drawing phase diagrams with Mathematica using THERMOCALC output

back

Mathematica is an amazing research tool that I swear by: I use it to prefly all algorithmic work for THERMOCALC, for example. But it is (a) expensive, (b) there is a steep learning curve, and (c) it is using a sledgehammer to crack a nut. The plan therefore is to replace the various Mathematica functions by free-standing programs—like DRAWPD. However, until that task is complete, the various Mathematica functions and examples are gathered in the "math" folder, for those of you who are brave enough to do battle with them.

The files in the "math" folder are:

myst.nb is a style file that needs to go in
Mathematica 4.1>Configuration>FrontEnd>StyleSheets
if you want the files to look as I intended them to look[1]

plotfun.nb contains all the Mathematica functions for drawing phase diagrams from manually-assembled THERMOCALC output

nck.nb contains the information for drawing many of the diagrams in White *et al.* (2001). It is a good place to look to see how to use "makeline" and "drawline".

delpt.nb contains the code and simple examples for using the ΔPT method of Worley & Powell (1999).

afm3.nb and **afm6.nb** contains the code and data for calculating the AFM compatibility diagram movies at 3 kbar and 6 kbar. (I have not checked this code under Mathematica 4.1. It might need a little work to run...)

Txm.nb contains the code and data for calculating the T-x pseudosection movie. (ditto warning...)

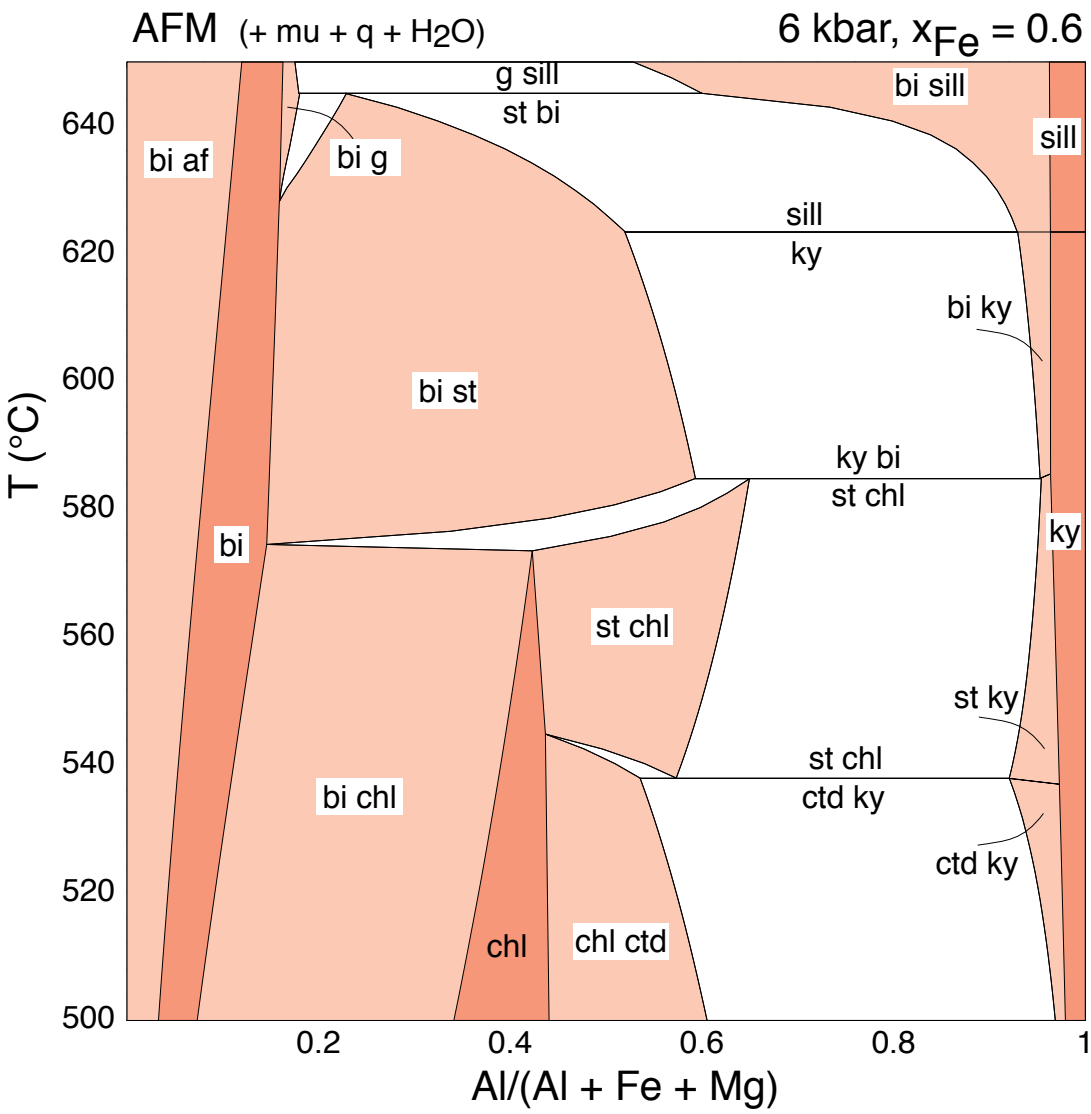
Ty.nb and **Px.nb** contains the code and data for calculating the T-y and P-x pseudosections. The labelled results follow. (ditto ...)

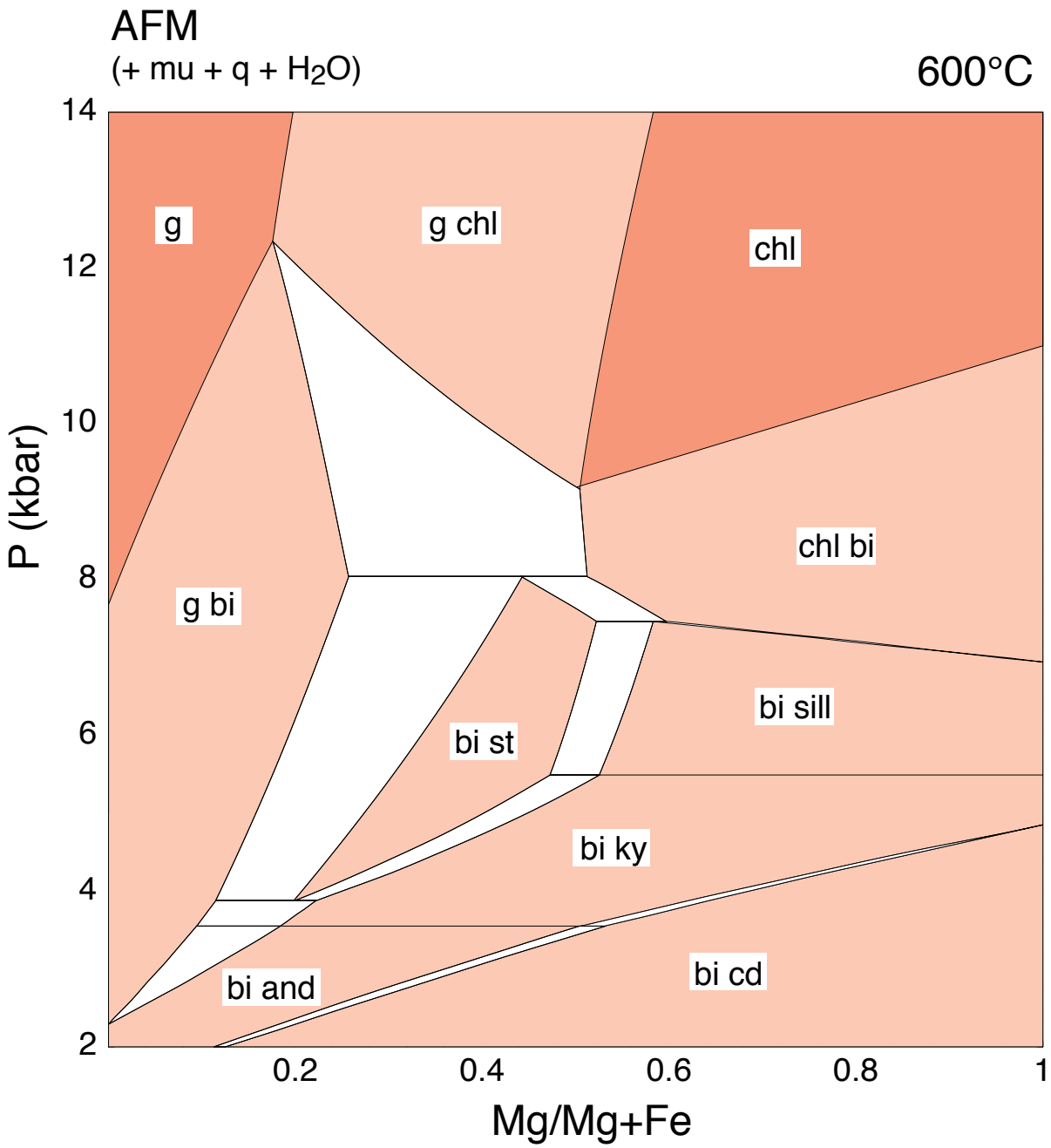
If you try calculating the same equilibria using the PDATA files on the CD-ROM, you will find (usually small) differences: the PDATA files used were from several earlier vintages.

If you are still using Mathematica 2.2, for example, I can make compatible Notebooks on request.

rp 6·5·01

[1] rp *is* a dalek...


AFM (+ mu + q + H2O)
6 kbar, xFe = 0.6
g sill
st bi
bi sill
sill
bi af
bi g
sill
ky
bi ky
bi st
ky bi
st chl
bi
ky
st chl
st ky
st chl
ctd ky
bi chl
ctd ky
chl
chl ctd
640
620
600
580
560
540
520
500
T (°C)
0.2
0.4
0.6
0.8
1
Al/(Al + Fe + Mg)


AFM
(+ mu + q + H2O)
600°C
P (kbar)
14
12
10
8
6
4
2
0.2
0.4
0.6
0.8
1
Mg/Mg+Fe
g
g chl
chl
chl bi
g bi
bi sill
bi st
bi ky
bi cd
bi and