

THERMOCALC Workshop 2001: Calculating Metamorphic Phase Equilibria

Practical 1

Questions 1 is easy if you are familiar with Schreinemakers analysis (the metastable part of reaction [i] lies between *i*-producing reactions...). But you will get to use DRAWPD for the first time.

1. Consider constructing the (familiar) part of the KFMASH (+ q + mu + H₂O) *PT* projection involving biotite (bi), chlorite (chl), garnet (g), staurolite (st) and kyanite (ky). Run “th dp1”, just hitting return when it asks for the phases you are interested in—so that it will use all of them in the list. It will calculate all the univariants around an invariant point. Consider 6 to 14 kbar, with an interval of 2 kbar. Now compare the contents of the “th dr” file you have produced with my “dr dp1” to see what I have done to prepare it for DRAWPD. Run my “dr dp1” through DRAWPD, then open the “drp1.ps” in Illustrator. It should look like Fig. 1, on which I have added labelling.

Do Schreinemakers on Fig 1, labelling the reactions with ‘out’ phases, and so on. To finish, run the invariant using “th dp1”, add its description from the “th dr” file, naming it, say, ‘i1’. Then replace the appropriate ‘begin’/‘end’ line limits for the univariants with ‘i1’ based on your Schreinemakers analysis. Then rerun DRAWPD. When you have opened the resulting “drp1.ps” in Illustrator, you can copy across the labelling from “p1” to finish the diagram.

2. Consider constructing the part of the KFMASH (+ q + ksp) *PT* projection involving biotite (bi), sillimanite (sill), garnet (g), cordierite (cd), orthopyroxene (opx), silicate melt (liq), and H₂O fluid (H₂O). It is a good guess that the amphibolite to granulite facies reaction in this system, bi + sill = g + cd + liq, will be stable over at least part of its length, so we start with that. The datafile to use is “th dp2”. There is the start of the DRAWPD datafile: “dr dp2”. It involves a *PT* window: 680° to 1000°C and 1 to 11 kbar.

We can observe, from a variance point of view, that invariants involving this set of phases will involve one phase out each. The best way of handling the Schreinemakers around each invariant is to sketch the positions of the univariants around the invariant on a piece of paper. When you put together the separate invariants, make sure that the stabilities of the reactions match... Of course, in general, not all of the invariants will be stable.

You can now add to “dr dp2”, and get DRAWPD to draw your final diagram. Although in relatively simple problems like this one you can assemble the DRAWPD information as you go, for more complicated ones, it is simpler to sketch up the whole thing first, then rerun the equilibria once you know what is going on.

(In this problem, we ignore muscovite, as well as having +ksp, so we will exclude from consideration that part of *PT* where mu+q is stable (lower *T* at higher *P*). We also ignore spinel. Apart from simplifying the prac, it is not very helpful considering spinel in KFMASH because its stability is so affected by Fe₂O₃.)

3. A straight Schreinemakers problem in a simple system to test your skills. In Fig 1, determine the stable equilibria, and label the fields with compatibility diagrams. It might help to go and read the Schreinemakers documentation on the CD-ROM. You can check what THERMOCALC reckons, by running “dr dp3” in mode 3 (having changed the “th prefs” file to allow access to mode 3).



