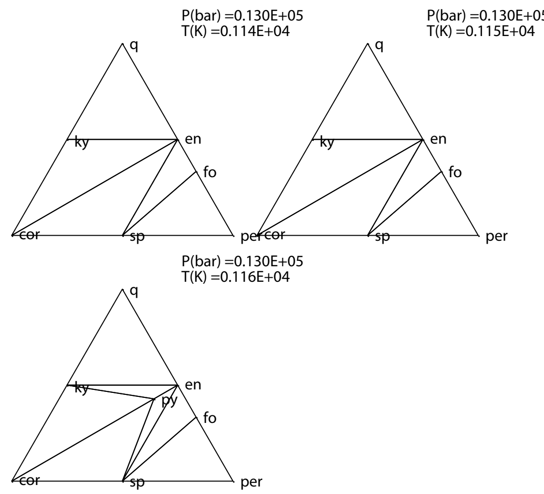
Perplex Tutorial Answers

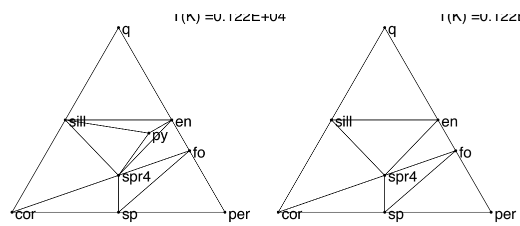
Files

The build files for each task are included with this distribution, as are PDF files of the diagrams that the students should produce.

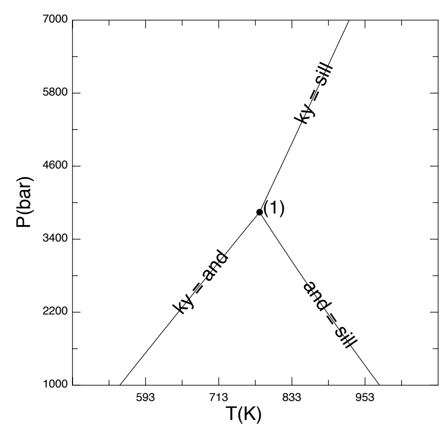
Tutorial I, Task 1



1. What are the reactions shown here?
   - From 1143K to 1153K, the reaction is the tieline-switching reaction of en + cor = ky + spr4
   - From 1153K to 1163K, the reaction is the appearance of pyrope at the expense of enstatite, kyanite and sapphirine (en + ky + spr4 = py).
2. Can you find either of them on the T-X(CO_2) diagram attached?
   - The first is the low-T, low-P reaction; the second is number 5.
3. Are they at the correct P-T-X(CO_2) conditions?
   - Yes, they are.
4. Examine your output; how is it different?
   - It should look like this at right. Lacking sapphirine, the first reaction cannot occur. Lacking an ex-ky-spr4 field, the second reaction is instead the appearance of pyrope from enstatite and corundum, en+cor=py.
5. Choose another reaction on the P-T diagram and calculate the diagrams.
   - [Depends on the reaction chosen; here's an example for spry+en+sil=py]

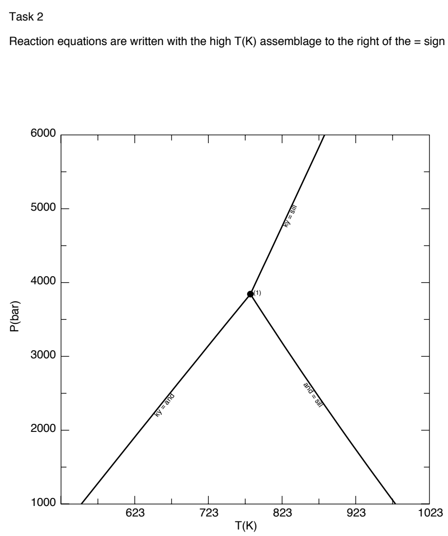


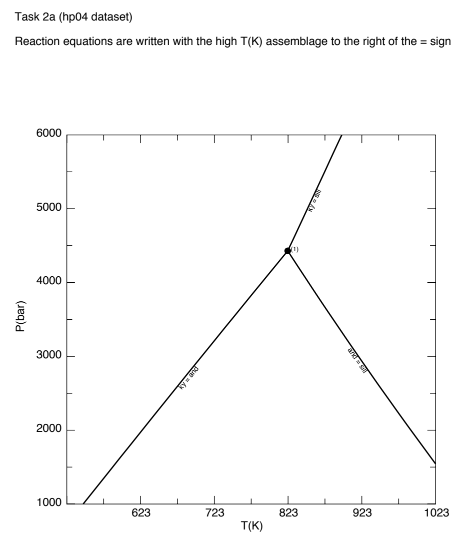
Tutorial II, Task 2



1. What determines whether you have corundum + kyanite or kyanite + quartz?
   - It depends on whether the system has more Al_2O_3 than SiO_2 or vice versa. There will in general be extra of one or the other beyond what is required to make Al_2SiO_5.
2. If kyanite is apparently stable at such low grades, why do we think of kyanite as being a high-pressure mineral?
   - At low pressures, none of the aluminum silicates typically form; instead we get hydrous Al-Si minerals like pyrophyllite or kaolininte.
3. What is the slope of the Ky-And reaction line (from the S & V values)?
   - $dP/dT = \Delta S/\Delta V = -9.32\ (J/K)\ /\ -0.742\ (J/bar) = 12.56\ (bar\ /\ K)$

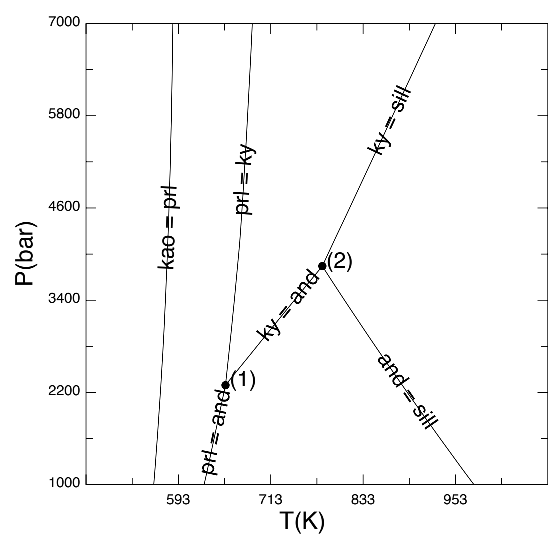
4. How do the coordinates of the invariant point compare to the commonly accepted (Holdaway & Mukhopadhyay, 1993) value of 3.75±0.25 kbar and 504±20 °C? Why might they be different?
   - The Perplex coordinates are 3.84 kbar and 507 °C, which are well within the uncertainties of the accepted values. However, they might be expected to differ somewhat because while the official values are based on experimental data for those minerals, the Perplex data set is an internally consistent one. This means that uncertainties in all the thermodynamic data get distributed over the whole data set so the values are consistent with each other. This will add uncertainty to any particular values and shift them somewhat from the best value determined by the experiments.
5. How does the diagram differ from the earlier one? How does the triple point compare to the Pattison (1992) value of 4.5±0.5 kbar and 550±35°C?
   - The diagram is similar, but the triple point is at 4.43 kbar and 550°C, within the error of the Pattison (1992) triple-point. (This is the primary difference between the hp02 and hp04 datasets.)





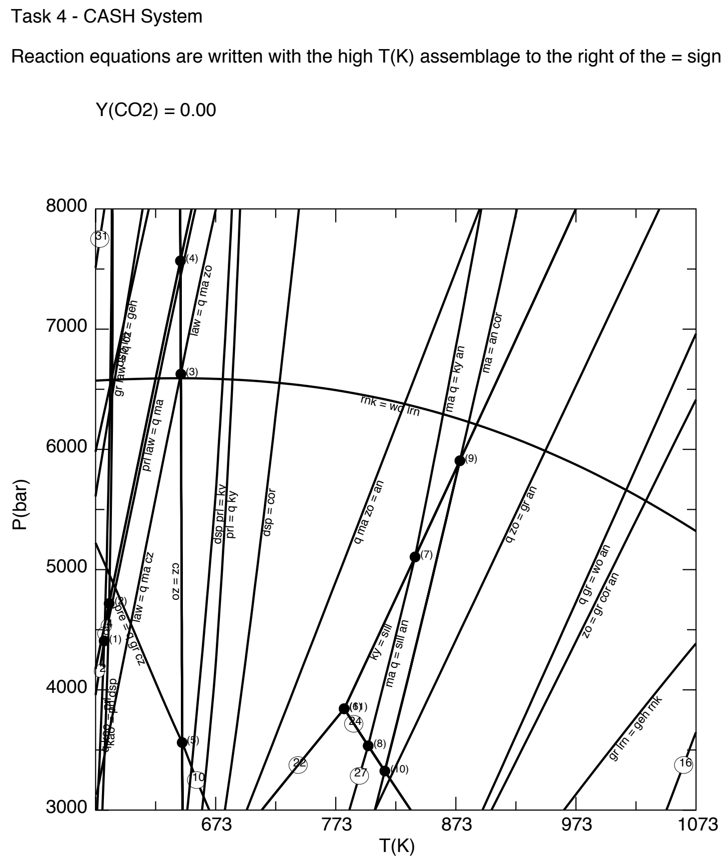
Tutorial II, Task 3

6. Looking at the set of minerals (you may wish to look up formulas), what is the key chemical difference in the system that allows pyrophyllite and kaolinite to form?
   - The presence of H_2O in the system allows these minerals, which have H in their structure, to form.
7. In the light of your new plot, do you have a different perspective on why we consider kyanite a high-grade mineral now?
   - Hopefully they now will say that it is that at low grades other minerals form to take up the Al and form sheet silicates and such.



Tutorial II, Task 4

8. Describe the setup you chose and what, if any, rock type your setup might apply to. Note particularly whether there are phases that are listed as multiple end-members, but are in reality solid solutions (e.g., diopside and hedenbergite).
   - There is no right answer to this question. The CASH system works out nicely (at right).

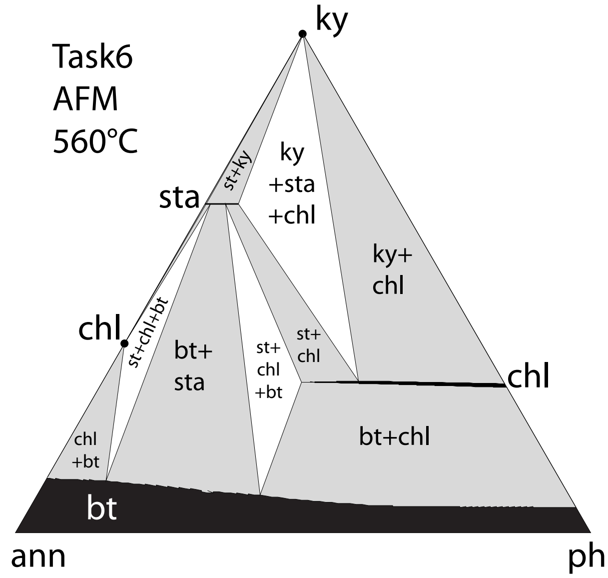


Tutorial III, Task 5

1. What do these phases have in common, and why are they listed here?
   - These are all SiO_2–Al_2O_3–K_2O–H_2O phases, and since we are projecting from those oxides, these may be present along with the phases in the plot.
2. What do the colors in the diagram correspond to?
   - The variance of the system. Lower variance (more phases) = lighter colors.
3. What changes across the Chl + St field from left to right? From top to bottom?
   - From left to right, the fraction of staurolite in the system decreases. From top to bottom, the fraction of staurolite in the system decreases, and both staurolite and chlorite become more Fe-rich.
4. How do the changes across a curved, steep boundary compare to changes across a horizontal field boundary?
   - Across a curved, steep boundary, a phase appears with an initially tiny amount or disappears after dwindling to a tiny amount. These boundaries are lines describing where the mode of a phase goes to zero. Across a horizontal boundary, there is a true reaction where one or more reactant phases is consumed to produce one or more product phases.
5. Write the full balanced reaction across the lower horizontal boundary, including the phases you are projecting from. You can assume that the projected phases are quartz, kyanite, and muscovite, and you can express a change in the composition of a phase as two separate phases, a reactant composition and a product composition.
   - 0.123 Chl_1 + 0.102 St + 0.116 Qtz + 0.224 H_2O = 0.1 Chl_2 + 0.52 Ctd + 0.4255 Ky

Tutorial III, Task 6

6. Describe qualitatively the changes occurring from 773 K through 833 K. If you wanted to get more specific knowledge of these changes, how would you use Perplex to figure those out?
   - Discontinuous reactions:
     - Staurolite appears
     - Chloritoid disappears and garnet appears
   - Continuous changes:
     - Biotite stability expands
     - Chlorite stability is reduced
     - Staurolite stability expands, then contracts
   - To get a more precise grasp of these, you could calculate more AFM diagrams at smaller temperature intervals.



7. Identify the discontinuous reaction(s) that must occur somewhere between 833 and 853 K.
   - Ky = Sil
   - Sta + Chl = Ky/Sil + Bio
8. Give the exact predicted composition (in terms of end-member proportions) of all minerals stable in this system at 5 kbar, 813 K, and X(CO_2)=0 in a rock whose bulk composition plots in the low-Al 3-phase triangle. You will have to look in the pseudocompound_glossary.dat file for compositions, and you might need to put the file in an editor to read the labels which probably overlap each other. In addition, you will need the composition of the end-members listed in the pseudocompound glossary – you must use the compositions listed in hp02ver.dat, not those you find anywhere else (including textbooks).
   - In the print file, this three-phase region is listed as: `Bi80_52 - fc92 - Ch24_70`
     - So we have a biotite, chloritoid, and chlorite, and we are projecting from quartz and muscovite, so they are present (and pure).
     - The biotite is: 42% annite, 10.5% phlogopite, 9.5% eastonite, and 38% siderophyllite
     - The chloritoid is: 92% Fe-ctd and 8% Mg-ctd
     - The chlorite is: 66.5% daphnite, 25% amesite, and 8.5% clinochlore

Tutorial IV, Task 7

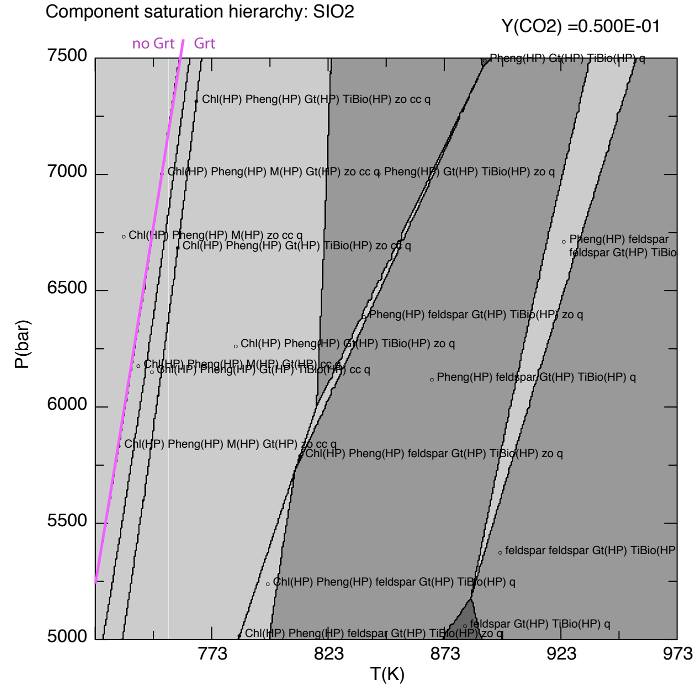
1. What precise phases are stable for this bulk composition at these conditions? Give their compositions (as chemical formulae) and volumetric abundances, normalized to 100%.
   - 11.9% K-feldspar – $(K_{0.99}Ca_{0.01})Al_{1.01}Si_{2.99}O_8$
   - 3.4% Anorthite – $(K_{0.03}Ca_{0.97})Al_{1.97}Si_{2.03}O_8$
   - 33.8% Garnet – $(Ca_{0.69}Fe_{1.21}Mg_{0.50}Mn_{0.60})Al_2Si_3O_{12}$
   - 17.0% Biotite – $K(Fe_{0.83}Mg_{1.89}Mn_{0.05}Al_{0.24})(Al_{1.24}Si_{2.76})O_{10}(OH)_2$
   - 33.9% Quartz

Tutorial IV, Task 8

2. Annotate the pseudosection (using Illustrator or Inkscape) to show the line that separates garnet-bearing rocks from non-garnet-bearing rocks.

Task 8 - Full pseudosection

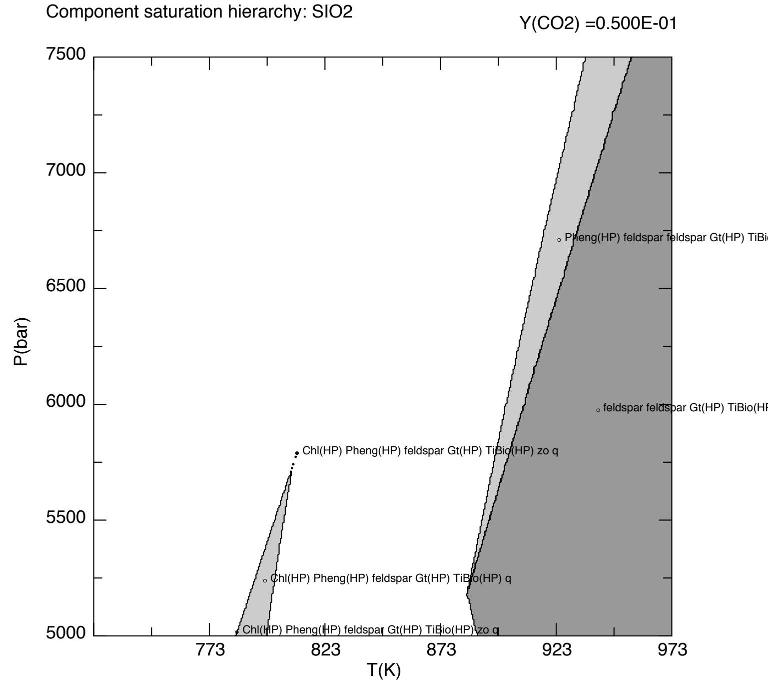
Component saturation hierarchy: SIO2



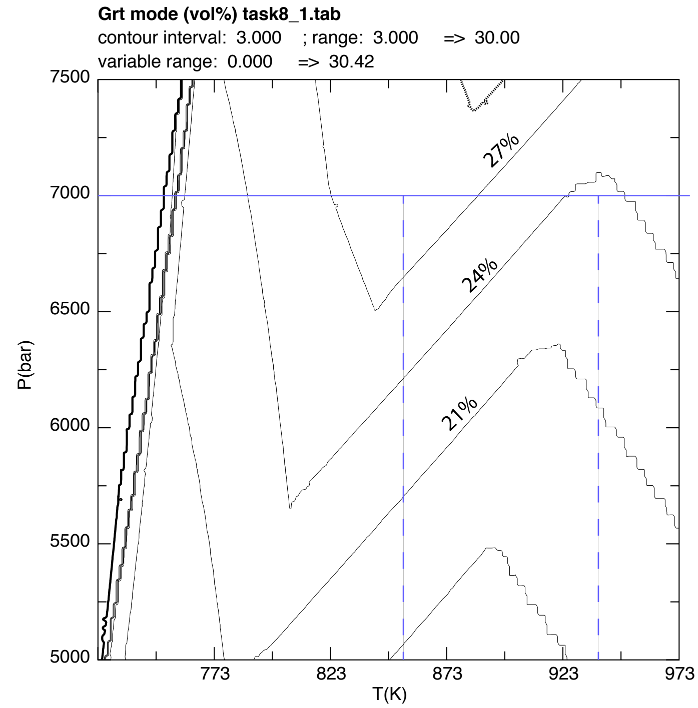
3. What additional mineralogical information would you need from the rock to determine in which of the fields it falls (presuming you know it falls in this region of P-T-X(CO_2) parameter space)? Turn this plot in. Be sure to give this plot an informative title, as well as the next two.
   - You would need to know what other phases are present, and how many feldspars are present.

Task 8 - Pseudosection showing Grt+Bt+Chl+Qtz+Fsp regions

Component saturation hierarchy: SIO2



4. Describe what would happen to garnet if the rock were to be isobarically heated at 7 kbar over this temperature range?.
   - Garnet grows up to 855K (28.26 vol%), then dissolves to 937K (23.64 vol%), then grows again to 973K (24.96 vol%).



5. Describe the MnO of the garnet during isobaric heating at 7 kbar. We know that garnet often has high Mn values in its core and smoothly decreasing Mn content toward the rim. Does that match with what the you would predict from this pseudosection? If not, how can you reconcile the two?
   - Garnet MnO begins at 0.999 formula units at 752K, then decreases along the path to 855K (0.727 formula units), then increases along the path to 937K (0.838 formula units), then decreases again along the path to 973K (0.796 formula units). This is generally consistent with the typical observations: highest Mn would be at the core, and lowest would be at the rim. However, there might be a spike in Mn in the middle, depending on how Mn was partitioned between garnet and matrix during the dissolution.
   - Regardless, this is not the typical cause of Mn zoning; rather the preferential partitioning of Mn into garnet during growth causes bell-shaped zoning, as early-formed garnet removes Mn from the system, changing the effective bulk composition of the rock as the garnet grows.