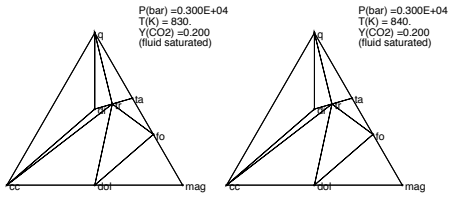
Perplex Tutorial Answers

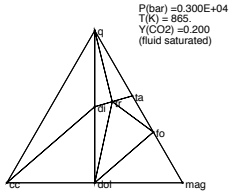
Files

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

Tutorial 1, Task 1

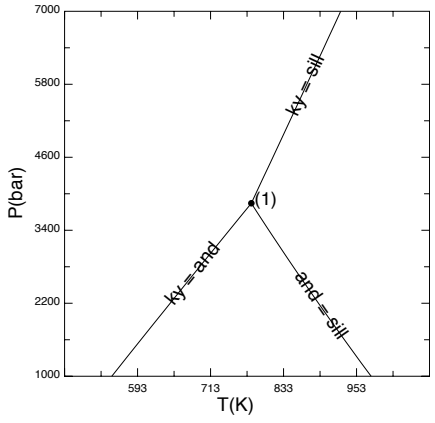
1. What are the reactions shown here?
   - From 830K to 840K, the reaction is the appearance of tremolite from the reaction q + ta + odo = tr.
   - Balanced: 4 SiO_2 + $Mg_3Si_4O_{10}(OH)_2$ + 2 $CaMg(CO_3)_2$ = $Ca_2Mg_5Si_8O_{22}(OH)_2$ + 4 CO_2
   - From 840 K to 865 K, the reaction is the appearance of diopside at the expense of quartz and dolomite (q + odo = di)
   - Balanced: 2 SiO_2 + $CaMg(CO_3)_2$ = $CaMgSi_2O_6$ + 2 CO_2
2. Can you find either of them on the T-X(CO_2) diagram attached?
   - They are number 19 and 28.
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. Note that diopside is already present at 830 K, and there is a different reaction between 840 and 865 K, the tieline-switching reaction of: tr + cc = di + dol





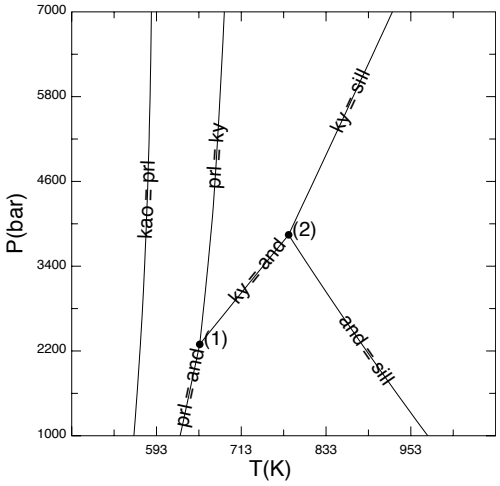
Tutorial 2, Task 2

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, 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.

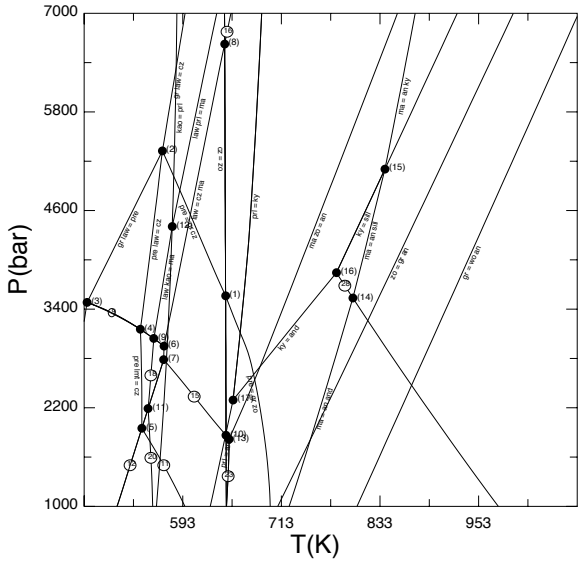


Tutorial 2, Task 3

5. 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.

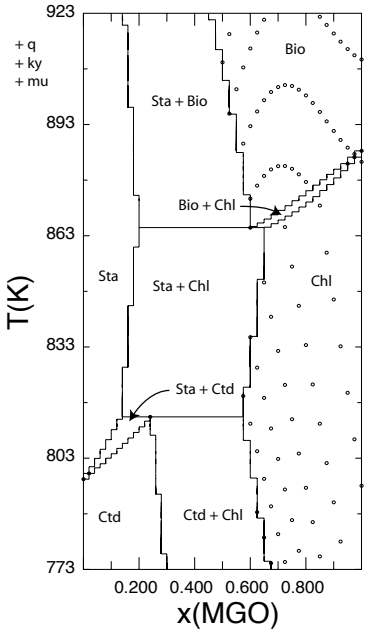
Tutorial 2, Task 4

- There is no right answer to this question. The CASH system works out nicely:



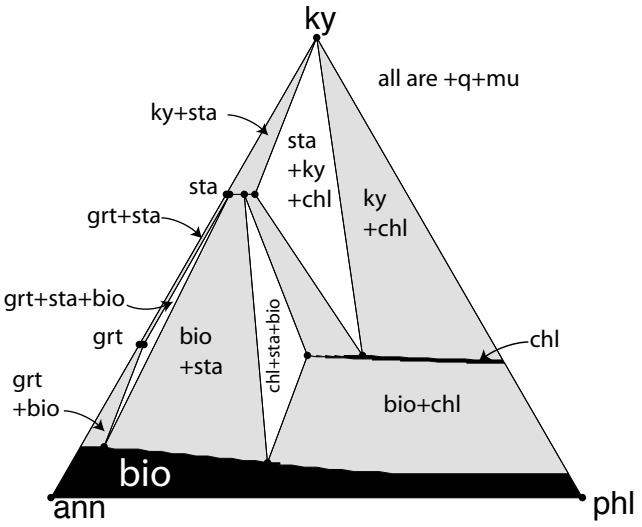
Tutorial 3, Task 5

1. What are the stable phases in each field on this T-XMgO plot? Print out the T-XMgO plot, and label each region with the stable phases. Indicate the minerals you are projecting from as well.
2. Give the full, balanced reaction (but without S and V), and its position in P-T-XMgO space.
   - 4 Ctd + 5 Ky = 1 St + 1.5 Q + 2 H_2O
   - P = 7 kbar, T = 797.356 K, X_{MgO} = 0



Tutorial 3, Task 6

3. (See diagram at right).
4. 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.



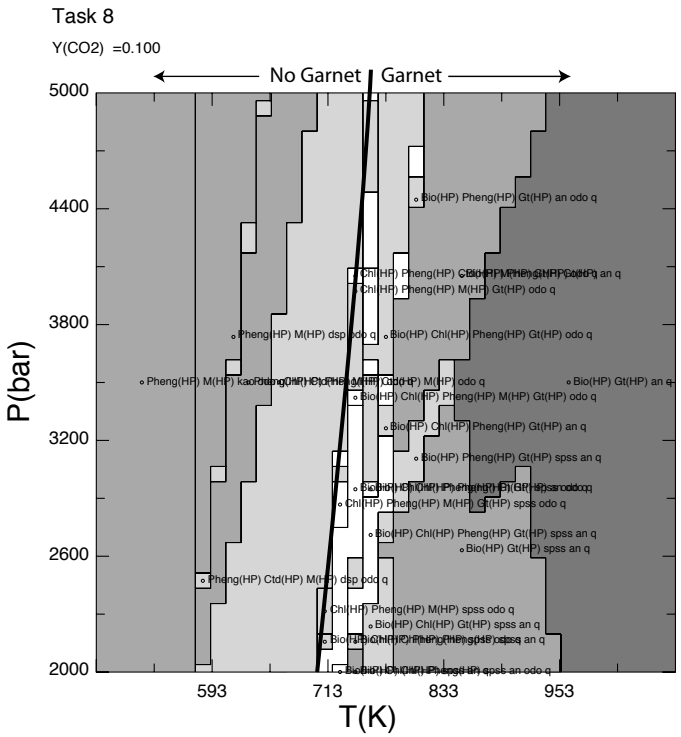
5. Identify the discontinuous reaction(s) that must occur somewhere between 833 and 853 K.
   - Sta + Chl = Ky/Sil + Bio
6. Give the exact predicted composition (in terms of end-member proportions) of all minerals stable in this system at 5 kbar, 813 K, and $X(CO_2)=0$ in a rock whose bulk composition plots in the low-Al 3-phase triangle. You will have to look in the pseudocompound_glossary.dat file for compositions.
   - 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

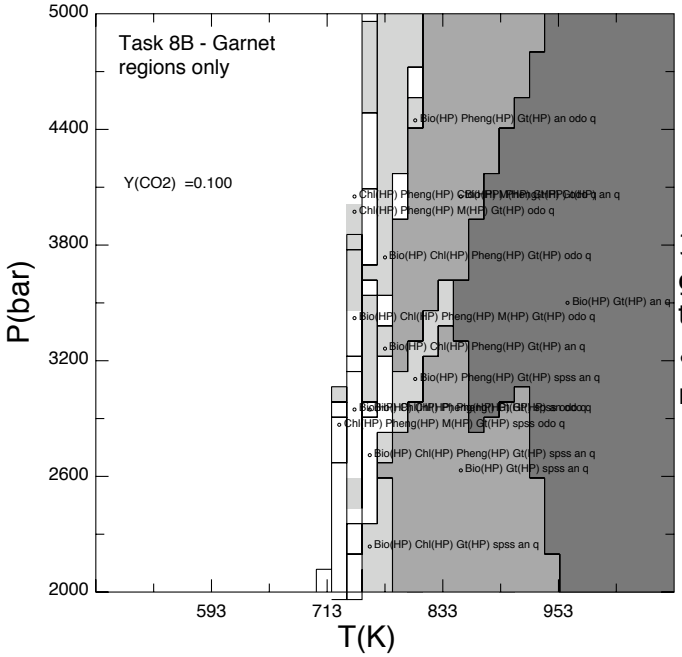
Tutorial 4, Task 7

1. What phases are stable for this bulk composition at these conditions? You will need to mathematically combine the pseudocompounds for each phase into a single phase composition, using the molar percents of each pseudocompound.
   - Biotite - $K(Fe_{1.22}Mg_{1.41}Mn_{0.11}Al_{0.26})(Al_{1.26}Si_{2.74})O_{10}(OH)_2$
   - Garnet - $(Ca_{0.49}Fe_{1.54}Mg_{0.37}Mn_{0.6})Al_2Si_3O_{12}$
   - Quartz
   - Anorthite

Tutorial 4, Task 8

2. Draw on the pseudosection the line that separates garnet-bearing rocks from non-garnet-bearing rocks. (Note that some of the tiny regions are artifacts of the coarse resolution of the calculations.) Turn this in.



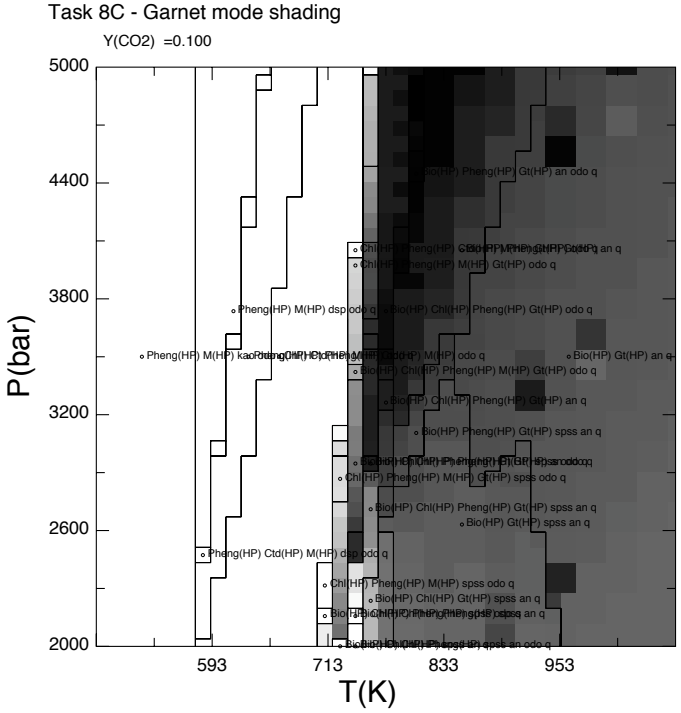


3.Turn this in, indicating at what pressure the garnet-forming reaction is found at the highest temperature.

•At the highest temperature, the garnet forming reaction occurs at 5 kbar.

4. Turn this in, indicating at what pressure garnet is made the fastest, under isobaric heating (assuming a constant heating rate)?

   • The fastest garnet growth occurs at the higher pressures, as shown by the sharp horizontal gradient in grayscale there.



5. Turn this in, and describe the MnO of the garnet during isobaric heating at 4 kbar. We know that garnet typically has high Mn values in its core and lower values toward the rim. Does that match with what the you would predict from this pseudosection? If not, how can you reconcile the two?
   - The common observation seems to disagree with this pseudosection. This is because the pseudosection omits consideration of the fractionation going on. As garnet grows, it strongly fractionates Mn, leaving the matrix depleted in Mn. Subsequent increments of garnet thus grow from a Mn-depleted environment and contain less Mn. Because the pseudosection calculates stability and composition **at equilibrium**, it cannot by itself account for varying effective bulk composition that results from this sequestration of Mn (and other elements to a lesser degree).