GLY 560 -- Thermodynamics and Isotopes in Geology **Name ____________________**

Thermodynamics and Isotopes in Geology, Problem 7

A preliminary phase diagram for the Al_2SiO_5 system

Kyanite, andalusite, and sillimanite are very important metamorphic minerals found in phyllites, schists, and gneisses. You can use thermodynamic data and equations to determine the location (in PT space) of phase boundaries for these minerals. For this exercise, we are assuming that ΔV^o_{rxn}, ΔH^o_{rxn}, and ΔS^o_{rxn} remain constant at high temperature and pressure.

Step 1:

form	formula	ΔH^o KJ/mol	ΔG^o KJ/mol	S^o J/mol/K	V^o cm^3/mol
kyanite	Al_2SiO_5	-2594.29	-2443.88	83.81	44.09
andalusite	Al_2SiO_5	-2590.27	-2442.66	93.22	51.53
sillimanite	Al_2SiO_5	-2587.76	-2440.99	96.11	49.90

Fill in the chart below with changes in H^o, G^o, S^o, and V^o for each reaction. Note, the units for ΔH^o_{rxn} and ΔG^o_{rxn} should be convert from KJ/mol to J/mol and ΔV should be converted from cm^3 to J/bar.

	ΔH^o_{rxn} (J/mol)	ΔG^o_{rxn} (J/mol)	ΔS^o_{rxn} (J/mol/K)	ΔV^o_{rxn} (J/bar)
1) kyanite → andalusite	____________	____________	____________	____________
2) andalusite → sillimanite	____________	____________	____________	____________
3) kyanite → sillimanite	____________	____________	____________	____________

Step 2:
Let's start with reaction (1); kyanite → andalusite.
First, calculate $\log K_{298}$ using the ΔG^{o}_{rxn} calculated above.

Next, use the equation discussed in class to calculate the equilibrium temperature. List your final answer in both K and ºC.

Use the Clapeyron Equation to calculate the slope of this reaction (bars/K).

If you add 200 K (or ºC) to the equilibrium temperature, what is the equilibrium pressure?

Plot these two points on the graph provided. Don't draw a line through them just yet….

Step 3:
Let's now examine reaction (2); andalusite → sillimanite.
First, calculate $\log K_{298}$ using the ΔG^{o}_{rxn} calculated above.

Next, use the equation discussed in class to calculate the equilibrium temperature. List your final answer in both K and ºC.

Use the Clapeyron Equation to calculate the slope of this reaction (bars/K).

If you <u>subtract</u> 100 K (or ºC) from the equilibrium temperature, what is the equilibrium pressure?

Plot these two points on the graph provided. You'll draw a line through them in a minute….

Note, this reaction (reaction 2) and the one before it (reaction 1), define the stable limits of andalusite. Now, starting at low pressure, draw lines through both sets of data and carefully extrapolate both lines (upward) until they just intersect.

Step 4:
Lastly, let's examine reaction (3); kyanite → sillimanite.
First, calculate $\log K_{298}$ using the ΔG^o_{rxn} calculated above.

Next, use the equation discussed in class to calculate the equilibrium temperature. List your final answer in both K and ºC.

Note that this temperature falls in the andalusite stability field. This is because kyanite and sillimanite would be *metastable* under these conditions. Kyanite and sillimanite are stable together at higher pressure (above the andalusite stability field). So we will calculate the slope of the reaction boundary and we will project this at pressures above the andalusite stability field.

Use the Clapeyron Equation to calculate the slope of this reaction (bars/K).

If you add 200 K (or ºC) to the equilibrium temperature, what is the equilibrium pressure?

If you add 400 K (or ºC) to the equilibrium temperature, what is the equilibrium pressure?

Plot these two points on the graph provided. Draw a line through them and extrapolate (downward) toward the intersection of the two previous reaction boundaries. Label the stability fields for kyanite, andalusite, and sillimanite.

Do your three reaction boundaries meet at a single point? __________

If not, are they close? Approximately how many ºC and bars off?

If so, what is the temperature and pressure of the triple point? T = __________ P = ___________