ESS 551 Assignment 3. Due October 23, 2006

1. Calculate ΔH, ΔS, and ΔG in expanding one mole of ideal gas at 25°C from 10 to 100 dm^3.

2. $CaCO_3$ (aragonite) → $CaCO_3$ (calcite) ΔG_m^0 (298K) = -800J, ΔV_m = 2.75 cm^3. At what pressure would aragonite become the stable form at 298K?

3. A thermodynamic study was made of the molecule tryptycene ($C_{20}H_{14}$) by measurements of heat capacity from 10 to 550 K. The compound melts at 527.18 K with ΔH_m = 7236 cal-mol^{-1}. The molar heat capacities were as follows:

Temp (K)	C_p (cal/deg-mol)
10	0.863
20	4.303
30	7.731
40	10.649
50	13.17
60	15.40
70	17.43
80	19.33
90	21.16
100	22.98
120	26.67
140	30.55
160	34.63
180	38.91
200	43.37
220	48.01
240	52.83
260	57.79
298.15	67.56
320	73.16
350	80.67
400	92.53
450	103.85
527.18	119.38
liquid	
527.18	130.86
530	130.90
550	133.45

1 Calorie = 4.1840 J. Plot the heat capacity versus temperature for this compound. Calculate the entropy for triptyciene at 298.15K and for the liquid at 550 K in units of J/mol-K.

4. Derive $C_P = -T(\partial^2G/\partial T^2)_P$ and $(\partial C_P/\partial P)_T = -T(\partial^2V/\partial T^2)_P$

5. Recent experiments show that forsterite converts to wadsleyite at 1500 K and 13.5 GPa. At 298 K and 1 atm, the entropy of this transition is 8.0 J mol^{-1} K^{-1} with a change in volume of 3.11 cm^3 mol^{-1}. Plot a line representing this phase boundary in P-T space. What assumptions do you have to make when using this data to construct phase boundary?

   Another way to obtain a phase boundary is to use measured enthalpies, measured volume changes with equations of states, and the above transition point to obtain an estimate of the entropy at those conditions. However, the enthalpy change has uncertainties: ΔH (975K) = 29.97 ± 2.84 kJ mol^{-1}.
   Then $\Delta G_{T,P} = \Delta H_T^0 - T\Delta S_T^0 + \int_0^P \Delta V_{T,P}\, dP$ is used to calculate the phase boundary by setting $\Delta G = 0$. The second and third terms in this equation relate directly to the Clapeyron slope while ΔH places it in the phase diagram much as does the location of one experimental data point (such as that given at the beginning of the problem). Using the uncertainties in ΔH given above, show how large the uncertainty in the placement of this transition in PT space becomes. Translate this to an uncertainty in depth using the pressure depth relationship in the PREM model (first week assignment).

   These are real experimental results and show some of the common problems in data interpretation.

6. Please state what goals you have in taking this course. This will help guide the course content if needed.