Exam #2 for Physical Chemistry for Energy Science

Department of Nuclear Engineering, Seoul National University
11/14/00 Thursday PM 2:30-4:00
90 min., closed book, one spike sheet(A4, both sides) allowed

1. **(15) Thermodynamic energy can be sum of each driving force x displacement.**

   1) For $dA = -SdT - PdV + \gamma dA + \mu dn$, explain meaning of each term on the right hand side.

   2) show that the condition for liquid drop and vapor at equilibrium is;

   $\mu^v = \mu^l + 2\gamma M/\rho r$

   where γ, M, ρ and r are surface tension, molar mass, density and the radius of droplet, respectively.

2. **(10) Describe two ways to obtain necessary data for constructing a phase diagram.**

3. **(20) For a pure substance,**

   1) Show that the molar internal energy can be determined from the following relationship:

   $$U - U_o = RT^2(\partial \ln z / \partial T),$$

   where U_o is U at O K.

   2) Derive an statistical expression for Standard Molar Gibbs Free Energy assuming the standard state of ideal gas.

5. **(15) Atoms in a single crystal are found to have energy states that are separated by a constant difference, ε_o.**

   1) Show that the partition function of the material is;

   $$z = 1/[(1-\exp(-\varepsilon_o/kT)]$$

   2) For the material described above, average energy per atom is

measured to be $a\varepsilon_0$ at a temperature Ta. Show that;

$$Ta=(\varepsilon_0/k)/\ln[1+(1/a)]$$

6. (10) What is the Gibbs paradox and how can you overcome it?

7. (15) $H_2(g)+\frac{1}{2}O_2(g)=H_2O(g)$. Assume all gases are ideal gases.

1) Under the constant volume and 25 °C, determine the heats of reaction.
2) Under the standard state and 25 °C, assume that the initial reactant mixture contains a 1:1 ratio of hydrogen and oxygen. What is the mole fraction of water vapor at equilibrium?
3) Under the standard state and 300 °C, assume that the initial reactant mixture contains a 1:1 ratio of hydrogen and oxygen. What is the mole fraction of water vapor at equilibrium?

8. (15) For the Haber synthesis,

$$\frac{1}{2}N_2+\frac{3}{2}H_2=NH_3$$

where $K_a=5.85\times10^{-4}$ at 1000 K and $K_a=2.04\times10^{-5}$ at 2000 K under standard state.

1) Calculate $\Delta_f H^{\ominus}_{298.15}$ of ammonia. Compare to the value given by Table 6.1. Why do they differ?
2) At 1000 K and 600 atm, determine K_p.
   NH_3: T_c=405.5 K, P_c=111.5 atm
   N_2: T_c=126 K, P_c=33.5 atm
   H_2: T_c=33 K, P_c=12.8 atm
3) At 1000 K and 600 atm, if the initial reactant mixture contains a 2:1 ratio of nitrogen and hydrogen, determine the mole fraction ammonia at equilibrium.