

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:

$$U - U_0 = RT^2 (\partial \ln z / \partial T),$$

where U_0 is U at 0 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_0 .

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

$$z = 1 / [1 - \exp(-\epsilon_0 / kT)]$$

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

measured to be $a\epsilon_0$ at a temperature T_a . Show that;

$$T_a = (\epsilon_0 / k) / \ln[1 + (1/a)]$$

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.

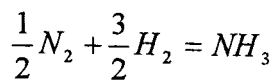
1) Under the constant volume and 25 °C, determine the heats of reaction.

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,



where $K_a = 5.85 \times 10^{-4}$ at 1000 K and $K_a = 2.04 \times 10^{-5}$ at 2000 K under standard state.

1) Calculate $\Delta_f H_{298.15}^\circ$ 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.

Handwritten calculations for problem 3:

$$\frac{10}{15} \quad \frac{10}{15}$$

$$\frac{2}{15} \quad \frac{3}{15}$$

$$\frac{10}{15} \quad \frac{10}{15}$$

$$\frac{2 \cdot 1}{1 + 2} = \frac{2}{3}$$

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