

Final Exam. for Physical Chemistry for Energy Science
Department of Nuclear Engineering, Seoul National University
6/19/07 Wednesday PM 6:00-9:00

Three hour, closed book, spike sheet (A4*2sides), data book allowed
Total 9 pages including data sheets.

1. (15) For ideal gas molecules with Maxwell velocity distribution, as follows;

$$F(v_x)dv_x = [m/(2\pi kT)]^{1/2} \exp(-mv_x^2/2kT) dv_x$$

Where the that v_x is the velocity in x-direction ranges from $-\infty$ to $+\infty$.

- (a) Show that the mean square momentum

$$\langle (mv_x)^2 \rangle = mkT$$

using the integration rule (attached).

- (b) Show that the variance (σ^2) of velocity becomes kT/m

- (c) Derive the expression on pressure, as function of velocity, number density and mass of molecules

- (d) Sketch the molecule population as function of translation energy

- (e) What is wrong with Maxwell's derivation?

$$\langle v_x^2 \rangle$$

$$\langle v_x \rangle^2 - \langle v_x^2 \rangle$$

$$p = \frac{nRT}{V}$$

2. (16) Suppose a diatomic molecular materials is invented at a laboratory of SNU for a fuel cell membrane and named as Gwanak. This has a melting point 449.5 C and boiling point of 989.8 C. Its gas at high temperature is consisted of di-atomic molecules that have the following electronic energy states, as measured by a laser spectroscopy;

Ground state: zero energy with 4-fold degeneracy

First excited state: $1/\lambda = 3400 \text{ cm}^{-1}$, 3-fold degeneracy

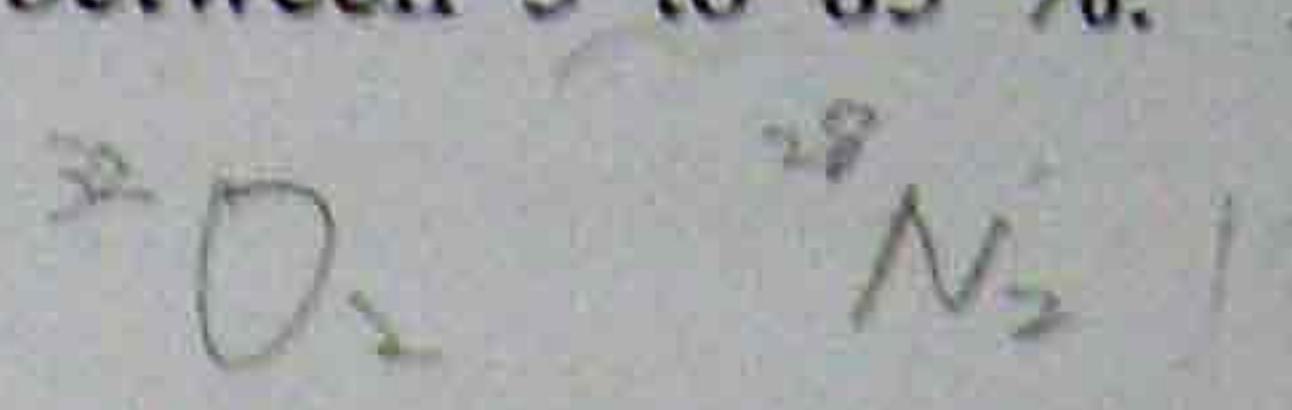
Second excited state: $1/\lambda = 4700 \text{ cm}^{-1}$, 1-fold degeneracy

Third excited state: $1/\lambda = 10500 \text{ cm}^{-1}$, 5-fold degeneracy

Hint: Its energy is related with wavelength by $E=hc/\lambda$

- (a) Calculate electronic partition function at 1000 K.
- (b) What is the specific heat of the gas at 1000 K if Gwanakium can be described by equi-partition principle?
- (c) Sketch specific heat of Gwanakium as a function of temperature from 0 K to 1000 K and explain key facts.
- (d) What is fraction of electrons at the lowest energy state at 1000 K ?

3. (9) An air-tight laboratory constructed with adiabatic walls has a 100 m³ of fixed volume, operating in air (21% oxygen 79% nitrogen) at one atm. pressure. A hydrogen cylinder with 140 liter of internal volume at 100 atm. was mistakenly left open to release all the gas completely overnight. Hydrogen explosion is possible when hydrogen mole fraction is between 5 to 85 %. Assuming ideal gas law, answer the following;

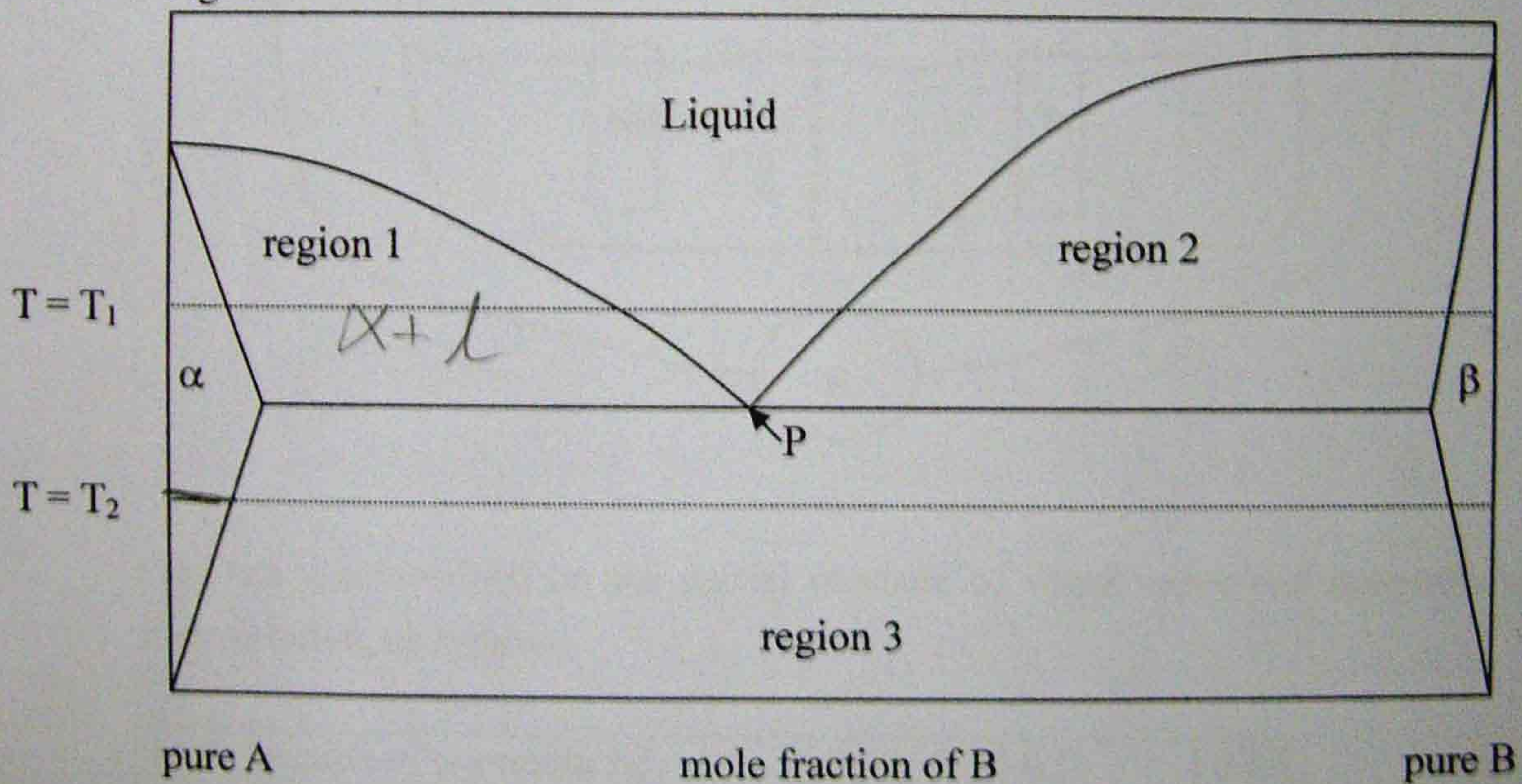


- (a) What is the partial pressure of hydrogen and oxygen after complete release at room temperature, but before explosion?
 (b) What is the maximum gas temperature after the explosion?
 (c) What is the mole fraction of each gas after the explosion.



4. (12) Gibbs free energy is available for most species in the form of database. For a mixture of two components, two solid states are possible, namely α and β . Then following phase diagram is constructed, as shown in Fig. 1;

Fig. 1.



- (a) What phase(s) exist in region 1, 2, 3, respectively?
 (b) Draw schematically Gibbs free energy of each phase as function of mole fraction of B at $T=T_1$.
 (c) At $T=T_2$, how can you determine the solubility of B in alpha phase?
 (d) What is the degree of freedom at the point P?

Handwritten notes on the right side of the page, including circled numbers 1 through 8 and some other scribbles.

Handwritten note: P

Handwritten equations and notes at the bottom of the page:

$$p + F = C + 2$$

$$F = C - p + 2$$

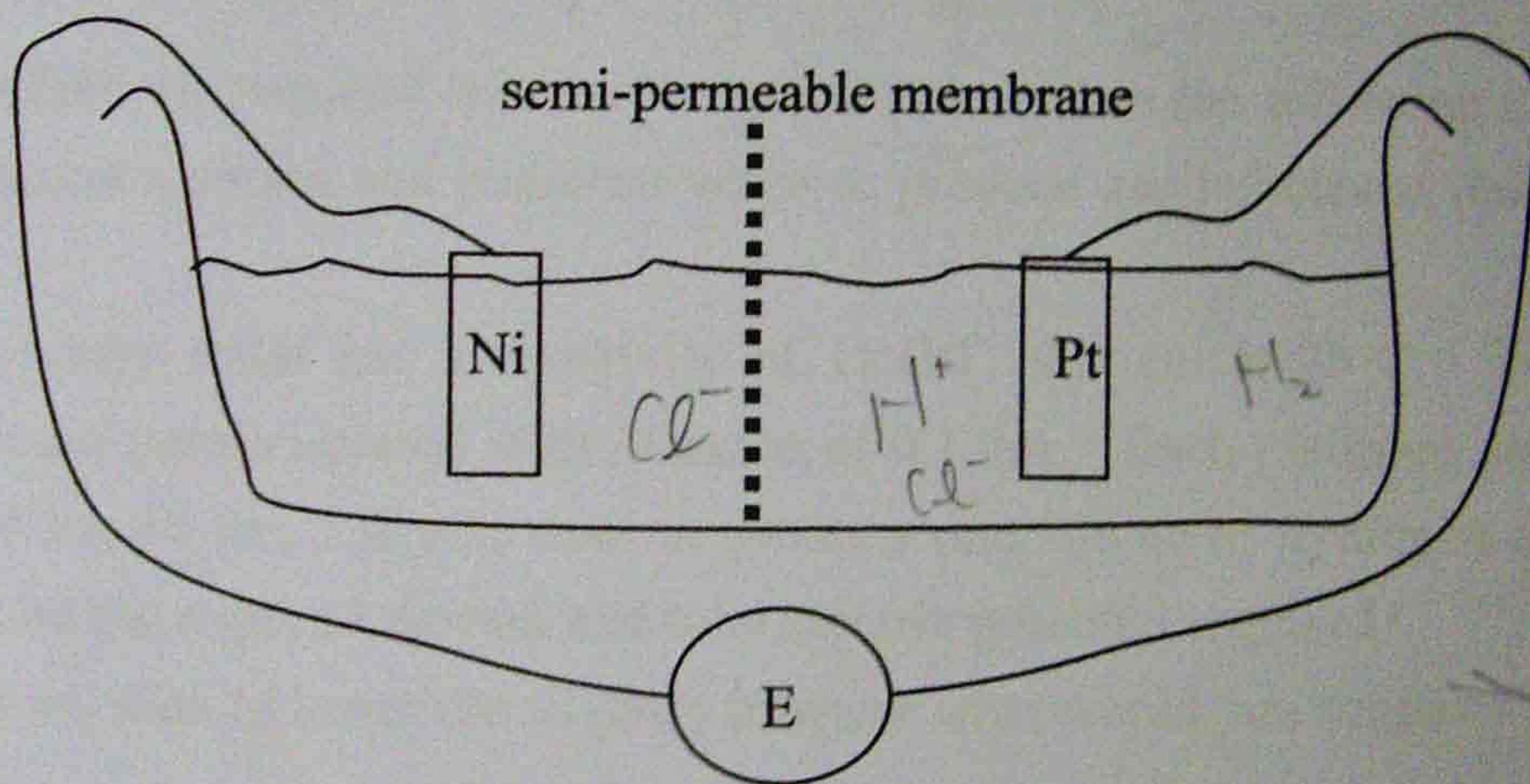
Notes: $n_{H_2O} - a =$, $a, \beta \quad C=2$, $p=3: a, l, \beta$

5. (9) The freezing point of water is depressed by 0.19°C with 0.11 mol/kg of NaOH.
- (a) Determine the degree of dissociation.
- (b) What is the solution pH?
- (c) Determine the change in Standard Gibbs Free Energy with ionization of NaOH.

6. (9) For the electrochemical cell of Fig. 2,
- left-side : $m_{\text{Ni}^{++}}=0.01\text{ mole/kg}$, $m_{\text{Cl}^-}=0.02\text{ mole/kg}$
- right-side : $m_{\text{H}^+}=0.01\text{ mole/kg}$, $m_{\text{Cl}^-}=0.01\text{ mole/kg}$, $P_{\text{H}_2}=2\text{ atm}$.

- (a) Write equilibrium reaction equation for each side
- (b) Determine mean ionic activity coefficient of ions in the left-side.
- (c) Determine the cell emf.

Fig. 2



7. (9) Data was obtained on the partial pressure of water vapor and ammonia above their solution, as follows;

| | | | | | |
|--------------------------------|------|------|------|-------|-------|
| mole fraction of ammonia | 0 | 0.05 | 0.1 | 0.15 | 0.2 |
| $P(\text{H}_2\text{O})$, torr | 18.6 | 17.6 | 16.5 | 15.5 | 14.5 |
| $P(\text{NH}_3)$, torr | 0 | 42.9 | 78.6 | 134.5 | 221.3 |

- (a) Plot all partial pressure as function of mole fraction of ammonia.
- (b) Determine Henry's law constant wherever applicable.
- (c) Determine if Raoult's law is applicable in any case.

8. (9) Gibbs-Duhem Equation is useful for evaluating the activity change of the first component from that of the second,

(a) Show that $d(\ln a_2) = - (x_1/x_2) d(\ln a_1)$

(b) For small change in activity, following approximation can be useful;

$$\Delta(\ln a_2) = - \langle x_1/x_2 \rangle \Delta(\ln a_1),$$

where $\langle x_1/x_2 \rangle$ denotes arithmetic average of the mole-fraction ratio during the logarithmic activity change, $\Delta(\ln a)$.

Then, the activity of CH₃OH and water is 0.254 and 0.717 respectively, when the mole fraction of CH₃OH is 0.1499. If the water activity is changed to 0.710 at the mole fraction of CH₃OH of 0.1501, what is the new activity of CH₃OH?

9. (12) Hydrogen can be produced by electrolysis of water.

(a) Write chemical reaction equation and determine GFE change per mole of water at 25 C.



(b) Determine the required minimum electric potential in the following cell consisted of two platinum sheets and platinum wires to produce gas bubbles at one atmosphere and 25 C.

(c) High purity water has a resistivity of 18×10^6 ohm-cm at 25 C. Two platinum electrodes are parallel-plated with distance of 0.1 cm. Each platinum plate has cross section of 2 x 10 cm. If you want to produce one 100 cc of hydrogen gas per hour, what will be the required current and total electric potential required?

(d) If you want to lower the IR-drop in water what would you suggest?

Fig. 3.

