Seoul National University

Department of Materials Science and Engineering

Midterm Examination 2 Physical Chemistry of Materials 2 November 26, 2012 Professor Won Ho Jo

- 1. Calculate the collision frequency per unit area for nitrogen gas at 25 °C and one bar. (10 pt)
- 2. If the temperature of a gas is doubled, by how much is the root-mean-square speed of the molecules increased? (10 pt)
- 3. The diffusion equation is valid when many elementary steps are taken in the time interval of interest, but the random walk calculation lets us discuss distributions for short times as well

as for long. Use the equation $P(x,t) = \left(\frac{2\tau}{\pi t}\right)^{\frac{1}{2}} \exp\left(-\frac{x^2\tau}{2td^2}\right)$ to calculate the probability of

being six paces from the origin (that is, at $x = 6\lambda$) after (a) four, (b) six, (c) twelve steps. (15 pt)

- 4. Many of concepts developed in kinetic theory can be applied to understanding the atmosphere. Because atmospheric air is comprised primarily of N_2 (roughly 78% by volume), approximate the atmosphere as consisting only of N_2 in answering the following questions:
 - (a) What is the single-particle collisional frequency at the sea level, with $T=298 \ K$ and $p=1 \ atm$? The corresponding single particle collisional frequency is reported as $10^{10} \ s^{-1}$.
 - (b) At the tropopause (11 km in altitude), the collisional frequency decreases to 3.16×10^9 s⁻¹, primarily due to a reduction in temperature and barometric pressure (i.e., fewer particles). The temperature at the tropopause is ~ 220 K. What is the pressure of N₂ at this altitude?
 - (c) At the tropopause, what is the mean free path for N_2 ?

(15 pt)

- 5. Evaluate the diffusion coefficient, the limiting molar conductivity, and the hydrodynamic radius of Zn^{+2} ion. The mobility (*u*) of the Zn^{+2} ion is $5.47 \times 10^{-8} \ m^2 s^{-1} V^{-1}$. (10 pt)
- 6. The temperature dependence of the acid-catalyzed hydrolysis of penicillin is investigated, and the dependence of k_1 on temperature is given in the following table. What is the activation energy and Arrhenius pre-exponential factor for this hydrolysis reaction?

Temperature (°C)	$k_1 (s^{-1})$
22.2	7.0×10^{-4}
27.2	9.8×10^{-4}
33.7	1.6×10^{-3}
38.0	2.0×10^{-3}

(10 pt)

- 7. For the second-order reaction of $A + B \xrightarrow{k_2} P$, the reaction is 60% complete in 60 seconds when $[A]_0 = 0.1 \, M$ and $[B]_0 = 0.5 \, M$.
 - (a) What is the rate constant for this reaction?
 - (b) Will the time for the reaction to reach 60% completion change if the initial reactant concentrations are decreased by a factor of 2?

(15 pt)

8. The Rice-Herzfeld mechanism for the thermal decomposition reaction of acetaldehyde (CH₃CHO) is

$$\begin{split} & \text{CH}_{3}\text{CHO} \xrightarrow{k_{a}} \text{CH}_{3} \cdot + \text{CHO} \cdot \\ & \text{CH}_{3} \cdot + \text{CH}_{3}\text{CHO} \xrightarrow{k_{b}} \text{CH}_{4} + \text{CH}_{2}\text{CHO} \cdot \\ & \text{CH}_{2}\text{CHO} \cdot \xrightarrow{k_{c}} \text{CO} + \text{CH}_{3} \cdot \\ & \text{CH}_{3} \cdot + \text{CH}_{3} \cdot \xrightarrow{k_{d}} \text{C}_{2}\text{H}_{6} \end{split}$$

Using the steady-state approximation, determine the rate of methane (CH₄) formation. (15 pt)