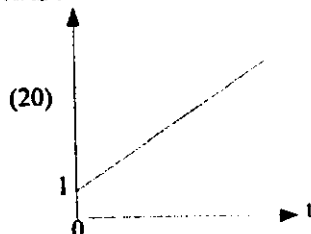


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學程別：

科目：物理化學

一、填充題：(每格2%)

1. 單一理想氣體分子的平均動能為 (1)，而在室溫下 He 與 O<sub>2</sub> 的平均運動速度 (root-mean-square velocity) 之比約為 (2)。
2. 凡得瓦爾常數與臨界壓力 P<sub>c</sub> 及體積 V<sub>c</sub> 之關係為 a = (3)，b = (4)。
3. 當 2 mole 的 H<sub>2</sub> 在外壓力 100 kPa 下，由 20 L 膨脹至 40 L 時，則 25 °C 等溫下，非可逆膨脹功為 (5) J，可逆膨脹功為 (6) J。
4. 根據定義，Gibbs 自由能與 Helmholtz 自由能之關係式為 (7)。
5. 米酒之酒精含量為 22 wt%，比重為 0.937。其莫爾體積濃度為 (8) M，而其凝固點較純水為 (9) (高/低)，其沸點較純水為 (10) (高/低)。
6.  $\int \frac{C_p}{T} dT =$  (11) (p constant)
7.  $\left(\frac{\partial G}{\partial T}\right)_p =$  (12)， $\left(\frac{\partial A}{\partial T}\right)_V =$  (13)。
8. 對於理想氣體， $\left(\frac{\partial G}{\partial T}\right)_V =$  (14)， $\left(\frac{\partial A}{\partial T}\right)_p =$  (15)。
9. 對於反應式  $H_{2(g)} + \frac{1}{2}O_{2(g)} = H_2O_{(g)}$ ，其反應平衡式為 K = (16)，若反應溫度提高，則 K 會變 (17) (大/小)，若反應壓力提高則 K 會變 (18)。
10. 對於碳酸鈣的分解： $CaCO_{3(s)} = CaO_{(s)} + CO_{2(g)}$ ，其自由度為 (19)。
11. 對於二級反應  $2A \rightarrow B$ ，其濃度 C 與時間 t 的關係如圖。請根據圖形填入縱座標。



二、計算題：

1. 1-Butene 的蒸氣壓與溫度 T (°K) 的經驗關係式為  

$$\log_{10} P (\text{atm}) = 5.5 - \frac{1343.5}{T} - 167.5 \times 10^{-5} T$$
 則根據 Clausius-Clapeyron 方程式，  
 (a) 其蒸發熱  $\Delta H_v$  與溫度之關係式為何？(2%)  
 (b) 在 1 atm 下，其沸點為何？(2%)
2. 已知在 1 atm, 100°C 時，水的蒸發熱為 2.26 kJ/g。則對於  $H_2O_{(l, 1 \text{ atm})} = H_2O_{(g, 0.5 \text{ atm})}$  此一程序，  
 (a) 其  $\Delta S$  為若干 kJ/°K/mol？(2%)  
 (b) 其  $\Delta G$  為若干 kJ/mol？(2%)
3. 在大氣中，室溫下水中溶氧的飽和濃度為 8.5 ppm (重量分率)，則氧在水中的亨利定律常數為若干 kPa·m<sup>3</sup>/mol？(2%)

三. Fill in the Blanks. 3% each blank. Although procedures are not essential, you may use the empty space for calculation.

1. Heptan-4-one is converted to ethylene with the aid of UV light. If  $9.45 \times 10^{19}$  photons generate  $2.36 \times 10^{19}$  ethylene molecules, then quantum yield = \_\_\_\_\_.
2. The mean-square displacement of particles undergoing 1 second of the Brownian motion (i.e., random walk) in the solvent is proportional to the  $n$ th power of the viscosity of surrounding solvent. Then  $n$  = \_\_\_\_\_.
3. The vibrational partition function of an ideal  $O_2$  gas molecule at an infinitely high temperature reaches a limiting value = \_\_\_\_\_.
4. The intermolecular energy of helium is equal to  $-A/r^6 + B/r^{12}$  ( $A, B$  are constants, and  $r$  = intermolecular distance). The equilibrium distance between two centers of molecules = \_\_\_\_\_.
5. In the band theory of solids, the band gap is defined as the energy difference between conduction and valence bands. Among three kinds of materials - metal, semiconductor and insulator, which one has the highest energy gap? \_\_\_\_\_.
6. The atomic electronegativity on the Pauling scale is 4.0 for fluorine and 2.1 for hydrogen, respectively. The dipole moment of HF molecules = \_\_\_\_\_ (in debye).
7. The measurement uncertainty in the position of a particle is inversely proportional to the uncertainty in the momentum of a particle. This statement is based on a rule called \_\_\_\_\_.
8. A reactant  $S$  is converted to a product  $Z$  with a catalyst. The reaction rate (in  $s^{-1}$ ) is given by  $5.0 \times 10^{-4}[S] / (5.8 \times 10^{-3} + [S])$ , where  $[S]$  is the concentration of  $S$  in  $M$ . When  $[S]$  is very high, the order of reaction = \_\_\_\_\_.
9. The infrared spectrum of CO has a strong peak at the wave number equal to  $2144 \text{ cm}^{-1}$ . The vibrational frequency of CO in  $s^{-1}$  = \_\_\_\_\_.
10. The (probability) distribution function of molecular speed for gas is  $f(u)$ , where  $u$  is molecular speed. The expression to define the mean speed is \_\_\_\_\_.

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12

Essay and Calculation Problems. 10% each problem. Write answers with detailed procedures.

四.

KCl (molar mass = 78.08 g/mol) crystallizes in a face-centered cubic lattice. The edge length of the unit cell is 627.8 pm (1 pm =  $10^{-12}$  m).

- What is the minimum diffraction angle for the fringes on the diffraction pattern of KCl? (The wavelength of x-ray = 154 pm) (4%)
- Is the lattice energy of 1 mole of KCl equal to the electrostatic potential energy between a  $K^+$  ion and a  $Cl^-$  ion times the Avogadro's number? Why? (3%)
- Given an unknown crystalline chloride compound, how do you determine its molar mass with the coupled experiment of density measurement and x-ray diffraction? Give the step(s) to reach the results. (3%)

五.

The wave function for the electron in H atom is

$$1/\pi^{0.5} (1/a_0)^{1.5} \exp(-r/a_0)$$

where  $r$  = distance between the electron and the nucleus

$a_0$  = Bohr radius

The wave function for the electron in  $H_2^+$  ion is

$$[(2+2S)\pi]^{-0.5} (1/a_0)^{1.5} \exp(-r_a/a_0) + [(2+2S)\pi]^{-0.5} (1/a_0)^{1.5} \exp(-r_b/a_0)$$

where  $S = (1+r_{ab}+r_{ab}^2/3)\exp(-r_{ab})$

$r_{ab}$  = distance between nuclei A and B

$r_a, r_b$  = distance between the electron and nuclei A and B, respectively

- In the  $H_2^+$  with  $r_{ab} = 2a_0$ , find the location where the electron appears most probably. Just write down the equations and do not try to solve them. (4%)
- How do you calculate the binding energy of the electron in H atom with the wave function given above? Just describe the method and do not try to write the equations. (3%)
- Show the molecular orbital diagram (i.e., the electron configuration) for  $H_2^+$ . (3%)