國立臺灣科技大學101學年度碩士班招生試題

系所組別： 材料科學與工程系碩士班甲組

科　　目： 物理化學

（總分為100分）

總分 100 分，共八大題。選擇題務必於答案卷內依序作答，在試題內作答者不予計分。

1. 選擇題：答案寫於答案紙內，其他方式作答不計分。

(18%) Choose the best answer in each problem. 3 points each. No penalty on the wrong guess. Be sure to answer all questions on the examination book, rather than problem sheet!

(1) According to transition state theory, the pressure dependency of reaction rate constant is determined by temperature and (a) activation energy, (b) activation of entropy, (c) Gibbs energy of activation, (d) activation enthalpy , (e) activation volume, of this process.

(2) The fast forward and backward rate constants in reversible, equilibrium reaction (e.g., the water hydrolysis) can be determined by (a) relaxation method in temperature change, (b) collision by molecular beam, (c) ultrafast laser,(d)electron emission with photoelectron spectroscopy, (e) magnetic resonance spectroscopy.

(3) The energy of hydrogen molecule as a function of the distance between two protons shows that, (a) energy of bonding state is always negative, (b) energy of antibonding state is always negative, (c) energy of bonding state has a minimum, (d) energy of antibonding state has a maximum, (e) bond length can be determined from the maximum in (d).

(4) As an atomic electron orbits around the nucleus, there is a relation in magnetism: :

(Magnetic moment vector) = (Constant) (Angular momentum vector)

Two vectors are in anti-parallel.

where constant is therefore equal to (a) e/2/m, (b) m/2/e (c) –e/2/m,(d) –m/2/e (e) em.

(where e= electron charge, m= electron mass.)

(5) While a particle in a three-dimensional well follows the time-independent Schrodinger equation for wave function F:

$$HF=EF$$

Where H is (a) a potential energy for particle, (b) total energy, (c) enthalpy function, (d) Hamiltonian operator, (e) operator for the square of the angular momentum.

(6) The probability density of a small particle in the first excited state (n=2) of an infinite (rigid) square well (with a width of L) has the maximum at the coordinate x= (a) L/6, (b)L/2, (c) L, (d) L/4 and 3/4L, (e) L/2 and L.

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2. Consider the reversible equilibrium reaction

A= B

Let k1= rate constant for the forward reaction = 1.0 /s

k2= rate constant for the backward reaction = 9.0/s

initial concentration of A = 1 M

initial concentration of B= 0 M

(1) Find the equilibrium concentration of A. (2%)

(2) Set up and solve the differential rate equation for A. Also present the A concentration in terms of time.(4%)

(3) At t= 10 s , calculate the the B concentration. (1%)

3. Molecular rotation can be tested with spectroscopy. The observed rotational frequency for the longest wavelength of carbon monoxide, CO, is 5.75E10 Hz. (note:"E" means a power function of 10)

a) Find the wavenumber (in the unit of reciprocal of cm) of this rotational transition. (2%)

b) Find the transition energy of the longest wavelength. (3%)

c) Find bond length of this molecule with given reduced mass , that is 1.14E-26 kg for a molecule.(5%)

*Useful Physical Constants

Planck constant= 6.626E-34 J-s

Gas constant= 8.317 J/K/mol

4. Please drive

(a) $\left(\frac{\partial G}{\partial T}\right)_P = -S$ and $\left(\frac{\partial G}{\partial P}\right)_T = V$ **(6 points)**

(b) $\left(\frac{\partial U}{\partial V}\right)_T = T\left(\frac{\partial P}{\partial T}\right)_V - P$ **(6 points)**

5. 1.95 molecules of an ideal gas with $C_{V,m} = 3/2R$ undergoes the transformations described in the following list from an initial state described by $T = 290$ K and $P = 1.0$ bar. Calculate q, w, ΔU, ΔH and ΔS for each process.

a) The gas is heated to 520 K at a constant external pressure of 1.0 bar. **(5 points)**

b) The gas is heated to 520 K at a constant volume corresponding to the initial volume. **(5 points)**

c) The gas undergoes a reversible isothermal expansion at 290 K until the pressure is half of its initial value. **(5 points)**

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6. At 298.15K, ΔG°_f(C, graphite) = 0, and ΔG°_f(C, diamond) = 2.9 kJ/mol. Therefore, graphite is the more stable solid phase at this temperature at P=P°=1 bar. Given that the densities of graphite and diamond are 2.25 and 3.52 kg/L, respectively, at what pressure will graphite and diamond be in equilibrium at 298.15K? (8 points)

7. (a) Can you express the "Clausius-Clapeyron Equation"? **(5 points)**

(b) What is Carnot Efficiency (Thermodynamic temperature scale) ? **(5 points)**

(c) One kind of the toy is called "Drinking Bird" (as shown in Fig. (i)). The glass contains the low boiling point liquid. When a kid holds the bottom, the body temperature can make the heat flow into liquid, then raise the liquid to H height (in Fig. (ii)). So, the neck of Bird is full of the liquid and falls down by the gravity (in Fig. (iii)). Fig. (iv) is the P-V diagram for process (i) to (iii). For the Drinking Bird, in process (i) to (iii) and apply answers in (a) and (b). Please write down the Carnot efficiency of the "Drinking Bird" in terms of T_1, T_2, g, $\triangle H_v$, R and ρ; where the heat of vaporization for the liquid at T_1 is $\triangle H_v$, g is a accelerate of gravity, R is gas constant and ρ is the density of a liquid. **(20 points)**

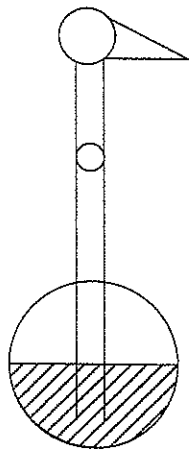

Fig. (i)

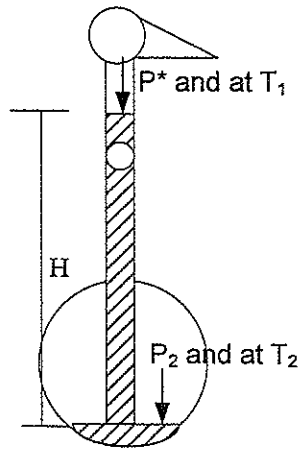

Fig. (ii)

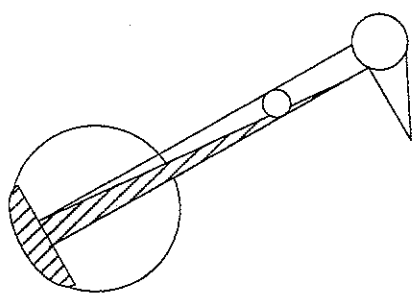

Fig. (iii)

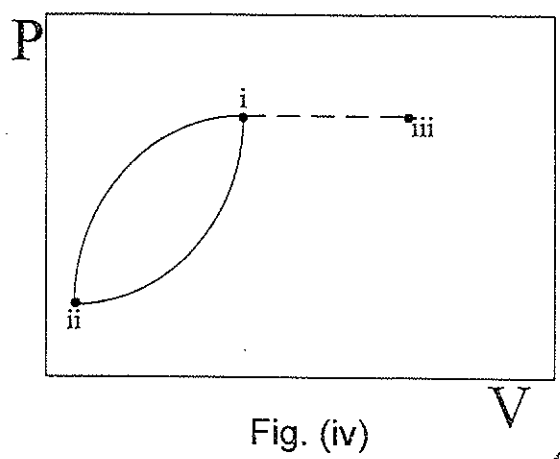

Fig. (iv)