國立台灣科技大學九十七學年度碩士班招生試題

系所組別： 高分子工程系碩士班丁組

科　　目： 物理化學

丁組：物理化學；共 9 大題，總分 100 分；請於答案卷內依序作答

1. One mole of an ideal gas with $C_V = 3/2R$ undergoes the transformations described in the following list from an initial state described by $T = 300$ K and $P = 1.00$ bar. Calculate q, w, ΔU, ΔH, and ΔS for each process.

a) The gas is heated to 450 K at a constant external pressure of 1.00 bar.(10%)

b) The gas is heated to 450 K at a constant volume corresponding to the initial volume. (10%)

c) The gas undergoes a reversible isothermal expansion at 300 K until the pressure is half of its initial value.(10%)

2. Consider the equilibrium $C_2H_6(g) \rightarrow C_2H_4(g) + H_2(g)$. At 1000 K and a constant total pressure of 1 atm, $C_2H_6(g)$ is introduced into a reaction vessel. At equilibrium, the composition of the mixture in mole percent is $H_2(g)$: 26%, $C_2H_4(g)$: 26%, and $C_2H_6(g)$: 48%.(10 %)

a) Calculate K_P at 1000 K.(2%)

b) If $\Delta H^\circ_{reaction} = 137.0$ kJ mol^{-1}, calculate the value of K_P at 298.15 K.(4%)

c) Calculate $\Delta G^\circ_{reaction}$ for this reaction at 298.15 K.(4%)

3. At 25°C, the combustion of ethanol in a fix-volume calorimeter produces 1300 kJ/mol of heat. (a) What is ΔU? (5%) (b) What is ΔH? (5%)
*The reaction is $C_2H_5OH_{(l)} + 3O_{2(g)} \rightarrow 2CO_{2(g)} + 3H_2O_{(l)}$

4. What are the asymptotic forms of Langmuir adsorption isotherm when the concentration [A] is (a) very low; (b) very high? (4%)

5. Complete the following relations: (a) $\left(\frac{\partial T}{\partial V}\right)_s$ (b) $\left(\frac{\partial G}{\partial P}\right)_T$ (c) $\left(\frac{\partial V}{\partial T}\right)_P$ (6%)

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CONSTANTS: *1 eV = 1.6E-9 J*

Planck constant= 6.63E-34 J-s

Bohr radius= 5.29E-11 m

Mass of electron= 9.11E-31 kg

Gas Constant= 8.31J/mole/K

Please indicate clearly units in the answers.

6. (10%)Vibrational levels of lithium bromide molecule (molar mass= 86.8) in its lowest state can be best approximated by a parabolic potential well, and have a force constant equal to 600 eV per square nm..

1) Find the characteristic vibrational frequency in the unit of cycle per second. (4%)

2) Find the lowest potential energy of this molecule. (3%)

3) Draw the REAL diagram of potential energy versus internuclear distance between Li and Br for the THREE lowest-value levels. (3%)

7. (10%) The hydrogen-like atom model may be applied approximately to the many-electron atoms. The first ionization energy of helium (atomic number= 2) is 24.6 eV. It is also known that the ionization energy of hydrogen is 13.6 eV.

1) Find the effective charge in the nucleus for the outer electron in He. Why is the effective charge lower than the atomic number? (3%)

2) If the wave function for the electron in H is A exp (-r/a), where A is a constant, r =the distance between the nucleus and the electron, and a =Bohr radius. Please indicate the method and equation to find the atomic radius of He, using this given expression and effective charge concept. (4%)

3) Find the second ionization energy of He. (3%)

8. (10%) Electrons in a transmission electron microscope were accelerated with electric field, and their kinetic energy is 10,000 eV.

1) Find the momentum of electrons. (3%)

2) Find the wave length of electron in motion, and compare it with that of x-ray (= 0.154 nm). (4%)

3) If neutrons, used to probe the materials structure, have the same kinetic energy as electron, what is their wave length? (3%)

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9. (10%) At 600 degrees centigrade, copper and gold forms a miscible solid solution. As the mole fraction of copper equals to 0.6, the activity coefficient of copper and gold is 0.536 and 0.246, respectively.
The saturated vapor pressure (P, in atm) of pure solid copper as a function of temperature (T, in K) is given by

$$\ln P = -40{,}920/T - 0.86 \ln T + 21.67$$

1) Find the partial pressure of copper in the vapor phase in equilibrium with the solid solution at 600 degrees. (3%).
2) Find the molar Gibbs free energy of mixing for this solid solution. (4%)
3) Find the molar enthalpy of vaporization for the pure copper at 600 degrees. (3%)