

國立臺灣科技大學

九十二學年度碩士班招生考試試題

系所組別：高分子工程系碩士班丁組

科目：物理化學

總分 100 分

- 1 a. Find the value of ΔG for 1.000 mol of ideal gas if it is isothermally pressurized from 1.000 atm to 3.000 atm at 298.15 K.

b. Find the value of ΔG if 1.000 mol of solid water is pressurized at 0.00°C from 1.000 atm to 20.000 atm. State any assumptions.

10%

- 2 At 35.2°C, the vapor pressure of pure acetone is equal to 344.5 torr, and that of pure chloroform is equal to 293 torr. At this temperature, a solution of 0.7090 mol of acetone and 0.2910 mol of chloroform has a vapor pressure of 286 torr and a mole fraction of acetone in the vapor of 0.8062.

a. Using Convention I, find the activity and activity coefficient of each component.

b. Find the Gibbs energy change of mixing and the excess Gibbs energy for the solution.

c. Henry's law constant for chloroform in acetone at this temperature is equal to 145 torr. Considering acetone to be the solvent, find the activity and activity coefficient for each component according to Convention II.

15%

- 3 The diffusion coefficient of bovine serum albumin in water at 20.0°C equals $7 \times 10^{-11} \text{ m}^2 \text{ s}^{-1}$.

a. Assuming the molecule to be spherical, estimate its radius.

b. Calculate the rms distance diffused in one direction in 30.0 min by protein molecules in water at 20°C.

the viscosity of water at this temperature is equal to

$$0.001002 \text{ kg m}^{-1} \text{ s}^{-1}. \quad D_2 = \frac{k_B T}{f}$$

10%

- 4 The particle in a one-dimensional box is sometimes used as a model for the electrons in a conjugated π -bond system (alternating double and single bonds).

a. Find the first three energy levels for a π electron in 1,3-butadiene. Assume a carbon-carbon bond length of $1.39 \times 10^{-10} \text{ m}$ and assume that the box is hard and consists of the three carbon-carbon bonds plus an additional length of $1.39 \times 10^{-10} \text{ m}$ at each end.

b. The molecule has four π electrons. Assume that two are in the state corresponding to $n = 1$ and that two are in the state corresponding to $n = 2$. Find the frequency and wavelength of the light absorbed if an electron makes a transition from $n = 2$ to $n = 3$.

$$E_n = \frac{h^2 n^2}{8ma^2}$$

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- 5 Identify each of the following statements as either true or false. If a statement is true only under specific circumstances, label it as false.
- The behavior of a molecule confined in a container will be noticeably different from the behavior of a free molecule.
 - Although part of the electronic energy in the Born-Oppenheimer approximation is kinetic energy, this energy acts as a potential energy for nuclear motion.
 - The orbital energy of a 4s subshell is always lower than that of a 3d subshell in the same atom.
 - The ground state of every inert gas corresponds to a filled valence shell.
 - The self-consistent theory can deliver the best possible orbital wave function for a multielectron atom.

5%

PHYSICAL CONSTANTS^a
(ROUNDED TO FOUR
SIGNIFICANT FIGURES)

Quantity	Symbol	Value
Speed of light in vacuum	c	$2.998 \times 10^8 \text{ m s}^{-1}$ (exact)
Permeability of vacuum	μ_0	$4\pi \times 10^{-7} \text{ N A}^{-2}$ (exact) $\approx 12.57 \times 10^{-7} \text{ N A}^{-2}$
Permittivity of vacuum	ϵ_0	$1/\mu_0 c^2$ (exact) $\approx 8.854 \times 10^{-12} \text{ C}^2 \text{ N}^{-1} \text{ m}^{-2}$
Planck constant	h	$6.626 \times 10^{-34} \text{ J s}$
$h/2\pi$	$\hbar$	$1.055 \times 10^{-34} \text{ J s}$
Elementary charge	e	$1.602 \times 10^{-19} \text{ C}$
Bohr magneton	μ_B	$9.274 \times 10^{-24} \text{ J T}^{-1}$
Nuclear magneton	μ_N	$5.051 \times 10^{-27} \text{ J T}^{-1}$
Rydberg constant	R_∞	$1.097 \times 10^7 \text{ m}^{-1}$
Bohr radius	a_0	$5.292 \times 10^{-11} \text{ m}$
Hartree energy	E_h	$4.360 \times 10^{-18} \text{ J}$
Electron mass	m_e	$9.109 \times 10^{-31} \text{ kg}$
Proton mass	m_p	$1.673 \times 10^{-27} \text{ kg}$
Neutron mass	m_n	$1.675 \times 10^{-27} \text{ kg}$
Deuteron mass	m_d	$3.344 \times 10^{-27} \text{ kg}$
Avogadro constant	N_A	$6.022 \times 10^{23} \text{ mol}^{-1}$
Atomic mass constant	m_u	$1.661 \times 10^{-27} \text{ kg}$
Faraday constant	F	$9.649 \times 10^4 \text{ C mol}^{-1}$
Gas constant	R	$8.315 \text{ J K}^{-1} \text{ mol}^{-1}$ $8.315 \times 10^{-2} \text{ L bar K}^{-1} \text{ mol}^{-1}$ $1.987 \text{ cal K}^{-1} \text{ mol}^{-1}$ $8.206 \times 10^{-2} \text{ L atm K}^{-1} \text{ mol}^{-1}$
Boltzmann constant	k	$1.381 \times 10^{-23} \text{ J K}^{-1}$
Acceleration due to gravity	g	9.80665 m s^{-2}

SOME NUMERICAL CONSTANTS
AND CONVERSION FACTORS

$\pi = 3.14159265$	$2.54 \text{ cm inch}^{-1}$
$e = 2.718281828$	453.6 g lb^{-1}
$\ln x = \log x / \log e = 2.30258509 \log x$	4.184 J cal^{-1} (exactly)
$101325 \text{ N m}^{-2} \text{ atm}^{-1}$	$1.602 \times 10^{-19} \text{ J eV}^{-1}$
$10^5 \text{ N m}^{-2} \text{ bar}^{-1}$	$10^{-3} \text{ m}^3 \text{ L}^{-1}$
$1.01325 \text{ bar atm}^{-1}$	$133.32 \text{ Pa torr}^{-1}$



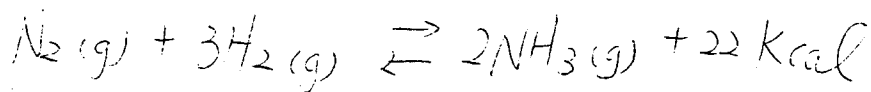
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6. 何謂 Le Chatelier's Principle? 試說明之。
根據此原理, 探討哈柏法 (反應式如下) 之最佳
反應條件為何? (10%)



7. 設有一 Unit Cell 加圖 1

其軸長分別為 a, b, c , 其角
度分別為 α, β, γ 加圖 2.

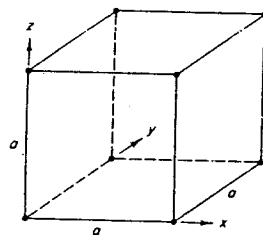


圖 1

若此 Lattice 之 System 為 Cubic
之時, 其軸長為 $a=b=c$, 而
其角度為 $\alpha=\beta=\gamma=90^\circ$. 若當

System 分別為 Tetragonal,

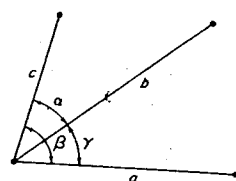


圖 2

Orthorhombic, Monoclinic, Triclinic 之時, 其軸長而
角度分別變化為何? 請作答 (10%)



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8. In the biological system, the synthesis of glutamine (Gln) from glutamate (Glu) is catalyzed by the enzyme glutamine synthetase according to the following equations:



which is coupled with



Therefore the complete reaction is



The ΔG° at 37°C are 15.7 and -31.0 kJ/mol for reaction (1) and (2), respectively.

- (a) Considering reaction (1) alone, what is the equilibrium value of $[\text{Gln}]/[\text{Glu}]$ if $[\text{NH}_4^+] = 1$ mM? (5%)
- (b) Write down the free energy expression of reaction (2). (5%)
- (c) Calculate the equilibrium constant of reaction (3)? (5%)
- (d) Considering reaction (2) alone, for a system with $[\text{ATP}] = 0.01$ mM, $[\text{ADP}] = 0.1$ mM, and $[\text{phosphate}] = 1$ mM, what is the direction of the reaction? (5%)
- (e) If a person had a fever of 40°C, what will the direction of reaction (3) be shifted? (5%)
- (f) If the concentrations of ATP, ADP, and phosphate are in equilibrium of reaction (2), will Gln be dissociated into Glu spontaneously? (5%)

