M.Sc. Sem II June 2018
Chemistry I (Rev.)

Q.P. Code : 35769

[2½ Hours] [Marks: 60]

Please check whether you have received the correct question paper.

N.B:
1. All questions are compulsory.
2. Figures to the right indicate full marks.
3. Use of nonprogrammable scientific calculator is allowed.

Useful constants

$c = 2{\cdot}998 \times 10^{8}\ ms^{-1}$	$e = 1{\cdot}602 \times 10^{-19}\ C$
$h = 6{\cdot}625 \times 10^{-34}\ Js^{-1}$	$m_e = 9{\cdot}110 \times 10^{-31} kg$
$R = 8{\cdot}314\ Jk^{-1}\ mol^{-1}$	$k = 1{\cdot}381 \times 10^{-23}\ JK^{-1}$
$N_A = 6{\cdot}022 \times 10^{23}\ mol^{-1}$	$1eV = 8{\cdot}06 \times 10^{3}\ cm^{-1}$
$N = 14, O = 16$	$1J = 6{\cdot}24 \times 10^{18}\ eV$

1. (A) Attempt **any two** of the following :
   i) Write the Schrodinger wave equation in terms of spherical coordinates. Why is it necessary to convert Schrodinger wave equation from Cartesian coordinates to spherical coordinates? Give the limits of variation for x, y, z and r, θ, ϕ. 4
   ii) Write the expressions for total wave function for 1s, 2s, 2p and 3d orbitals of hydrogen atom. 4
   iii) What are radial probability distribution curves? What information is obtained from these curves? Sketch qualitatively the radial probability distribution curves for 1s, 2s and 2p orbitals. 4
   iv) For an ethylene molecule, set up and solve Huckel determinant equation. Show the molecular orbitals energy levels and indicate HOMO, LUMO in ethylene molecule. 4

   (B) Attempt **any one** of the following :
   i) Calculate the energy of the third rotational energy level in the molecule of nitric oxide. The internuclear distance in the molecule is 0·11nm. 4
   ii) Find the most probable distance of an electron from the nucleus of hydrogen atom in 1s and 2s states. 4

2. (A) Attempt **any two** of the following :
   i) What is fugacity? How can it be evaluated from van der waal's equation of state. 4
   ii) Define partial molal volume. How is it determined by intercept method? 4
   iii) Write the BET isotherm equation and explain the terms involved in it. Give its significance. 4
   iv) What is ATP? Give its structure. Write any one biochemical reaction involving ATP with reference to changes in free energy. 4

   (B) Attempt **any one** of the following :
   i) Calculate the chemical potential, over and above standard chemical potential, of oxygen present in a mixture when the partial pressure is 4
   (a) 2 atm (b) 10 atm

Turn Over

ii) 4 litres of an ideal gas (molar mass 16) and 1 litre of another ideal gas (molar mass 40) each at 1 atm and 300K are mixed isothermally in a vessel of 3 litres capacity. Find ΔG_{mix}. 4

3. (A) Attempt **any two** of the following :

i) Derive the parabolic rate law for the reaction of a gas on the surface of solid particles. 4

ii) Explain the 1) Lineweaver-Burk's plot and 2) Eadie-Hoftsee's plot which is used for the analysis of the rate data of enzyme catalysed reaction. 4

iii) Discuss the kinetics of enzyme inhibition action by non-competitive inhibition method. 4

iv) Derive Hammet's equation of linear free energy relationship. 4

(B) Attempt **any one** of the following :

i) The following data applies to an enzyme-catalysed reaction :- 4

[S] mol dm^{-3}	Rate, R mol dm^{-3} s^{-1}
$2{\cdot}5 \times 10^{-4}$	$2{\cdot}3 \times 10^{-4}$
$5{\cdot}0 \times 10^{-3}$	$7{\cdot}8 \times 10^{-4}$

Using Michaelis-Menten's equation, calculate the Michaelis constant K_m and the limiting rate V.

ii) Predict the effect of ionic strength on the rate constant for each of the following reactions:- 4

1. $[Co(NH_3)_5Br]^{2+} + Hg^{2+} \rightarrow$ Products
2. $CH_2ICOOH + CNS^- \rightarrow$ Products
3. $[PtCl_4]^{2-} + OH^- \rightarrow$ Products
4. $H_2O_2 + Br^- + H^+ \rightarrow$ Products

4. (A) Attempt **any two** of the following :

i) Explain the phase diagram of a two component system involving formation of a compound with congruent melting point. 4

ii) Derive an equation relating to the number of vacancies found under equilibrium in a monoatomic crystal at a constant temperature to the average energy required to create one vacancy. 4

iii) Explain the phase diagram of a two components system of solid-gas involving formation of hydrates of copper sulphate. 4

iv) Draw and discuss the phase diagram of a three component system consisting of three pairs of partially miscible liquids. 4

(B) Attempt **any one** of the following :

i) Calculate the number of phases, the number of components and the number of degrees of freedom in the following system. 4

1. $N_2(g) + 3H_2(g) \rightleftarrows 2\,NH_3(g)$
2. Sodium chloride solution.

ii) If the average energy required to create a vacancy in a metal was 1 eV, calculate the ratio of vacancies in the metal at 1000K and 500K. Given $K_B = 8{\cdot}625 \times 10^{-5}$ eV/K. 4

5. Attempt **any four** of the following :

(a) Give the characteristics of real solutions.

(b) Show that enthalpy of ideal mixing of gases is zero.

(c) Write the expression for 'theta' equation, 'R'-equation and 'phi' equation for separatio variables of Schrodinger wave equation.

(d) Explain the significance of magnetic quantum number.

(e) Discuss the various factors affecting reactions in solids.

(f) Discuss the kinetics of regulatory enzymes with the help of Hill's equation.

(g) Explain why the various tie lines within the binodial curve are parallel neither to the sid triangle nor to each other.

(h) What are point defects? Explain Frenkel defects.
