This question paper contains 4 printed pages]

AY—150—2018

FACULTY OF SCIENCE

M.Sc. (First Year) (First Semester) EXAMINATION

MARCH/APRIL, 2018

(CBCS Pattern)

CHEMISTRY

Paper III (CH-413)

(Physical Chemistry—I)

(Friday, 13-4-2018)

Time: 10.00 a.m. to 1.00 p.m.

Time—3 Hours

Maximum Marks—75

- N.B. := (i) Attempt AII questions.
 - (ii) Use of log-table and calculator is allowed.
 - (iii) Solve Q. No. 5(A), MCQ in one attempt only.

Given: (1) $h = 6.626 \times 10^{-34} \text{ Js}$

- (2) Mass of electron, $m_e = 9.109 \times 10^{-31} \text{ kg}$
- (3) $C = 3 \times 10^8 \text{ m/s}$
- (4) $R = 8.314 \text{ Jk}^{-1} \text{ mol}^{-1}$
- (5) Boltzmann constant, $K = 1.38 \times 10^{-10}$ erg./deg./mole.
- 1. Solve any three:

15

- (a) Use Schrödinger equation in Laplacian operator form to explain Eigen-values and Eigen functions.
- (b) Explain the ternary system containing two pairs of partially miscible liquid components with phase-diagram.
- (c) Calculate the ionic strength of:
 - (i) $2MZnSO_4 + 2MZnCl_2$ and
 - (ii) 0.05 aluminium phosphate.

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- (d) Write short notes on:
 - (i) Schottky defects
 - (ii) Frenkel defects.
- (e) Write an account on Wein effect.
- 2. Attempt any three our of five:

(a) Define Lattice energy. Explain Born-Haber cycle for the formation of NaCl. How is it useful to stability or crystal structure?

15

7

(b) Prove that:

$$\left[\hat{s}^2,\,\hat{s}_z\right]=0.$$

- (c) What are partition functions? Explain its any two applications.
- (d) Derive the Lipmann equation of surface excess phenomenon.
- (e) Explain Recapitulation of phase rule to ternary systems and the terms involved it.
- 3. Solve:
 - (a) For a particle in 3D-box, show that:

(i)
$$\mathbf{E}_n = \frac{h^2}{8ml^2} \left[n_x^2 + n_y^2 + n_z^2 \right]$$
 and

$$(ii) \qquad \psi_n = \frac{2\sqrt{2}}{\sqrt{V}} \left[\sin\left(\frac{n_x \pi x}{l}\right) \sin\left(\frac{n_y \pi y}{l}\right) \cdot \sin\left(\frac{n_z \pi z}{l}\right) \right].$$

Or

Write an account on first order and non-degenerate perturbation theory.

(b) Calculate the wavelength of light absorbed in nm when an electron transition takes place from first energy level to second in one dimensional box of width 10 Å. What is the effect of increase in length of box?

Or

What is normalisation of wave function? Show that 1s-wave function of H-atom is,

$$\psi_{1s} = \psi_{100} = \frac{1}{\sqrt{\pi} \, a_0^{3/2}} \, e^{-r/a_0}$$

normalised where, a_0 is Bohr's radius and $dr = r^2 dr \sin \theta \ d\theta$ d.

4. Solve:

(a) Define fugacity of a gas and describe a method of its determination at any pressure from the P-V-T data.

Or

State Debye-Hückel limiting law. How is it experimentally verified? An aqueous solution at 25° C is 0.005 molal in sodium chloride and 0.008 molal in potassium sulphate. Calculate the activities of Na⁺ and SO_4^{--} -ions.

(b) For ideal solutions, the value of activity coefficient is unity; explain it. Describe the solubility method for determination of activity of electrolytic solutions.

Or

Explain the calculations of thermodynamic properties in terms of partition functions. Calculate the vibrational partition function of molecular hydrogen at 300 K, assuming it to be harmonic oscillator. (Given $w = 4405 \text{ cm}^{-1}$).

5. (A) Select the *correct* alternatives:

5

- (i) The wave functions ψ_n and ψ_m are said to be orthogonal if :
 - (a) $\int \psi_n \psi_m \, d\Gamma = 1$
 - $(b) \qquad \int \psi_n \psi_m \, d\Gamma = 0$
 - $(c) \qquad \int \psi_n \psi_m = -1$
 - (d) None of the above

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	(ii)	In three component systems, Tie lines are not used in the region of:
		(a) 1-phase
		(b) 2-phase
		(c) 3-phase
		(d) Both (a) and (c)
	(iii)	In Grand-canonical ensemble, the constants are:
	(111)	(a) E, V, N
		(b) T, V, N
		(c) T, V, μ
		(d) None of the above
	(iv)	Generally, Transition metal compounds exhibit:
	(IV)	(a) Metal excess defects
		(b) Metal deficiency defects
	150	(c) Stoichiometric defects
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		(d) None of the above
	(V)	The intercept of the plot Λ_c versus $\sqrt{c_i}$ extrapolated to zero concentration is :
		(a) Λ_0
920 C C 20 9		(b) Λ_v
		(c) Δ_{∞}
		(d) Both (a) and (c)
(B)	Write	short notes on any two:
	(a)	Eutectic systems containing two solid and a liquid components
	(<i>b</i>)	Stern's theory
	(c)	Zeeman effect
	(<i>d</i>)	Paulis exclusion principle.
AY—150—2	2018	4

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AY—150—2018