



MEB-4710 Seat No. _____

M. Sc. (Sem. I) Examination

November / December - 2018

CHN - 403 : Physical Chemistry : Paper - III

Time : 3 Hours]

[Total Marks : 70

Instructions :

- (1) Each question carries 14 marks.
- (2) Figures to the right indicate marks of the question.

1 (a) Answer any **two** of the following : 10

- (1) Set up and solve the Schrodinger wave equation for one-dimensional simple harmonic oscillator.
- (2) Discuss the applications of variation method taking the example of multi electron system.
- (3) Discuss the application of perturbation theory of helium atom.

(b) Answer any **one** of the following : 4

- (1) Write a note on "The rigid rotor".
- (2) Discuss the various postulates of wave mechanics.

- 2 (a) Answer any **two** of the following : 10
- (1) Explain the Huckel theory of conjugated system.
 - (2) Discuss spin angular momentum.
 - (3) Note on Eigenfunctions and Eigenvalue for angular momentum operator.
- (b) Answer any **one** of the following : 4
- (1) Discuss Pauli's exclusion principle.
 - (2) Short note Slater-Condon parameters.
- 3 (a) Answer any **two** of the following : 10
- (1) Define Zeroth law, first and second law of Thermodynamics.
 - (2) Explain : any one method for determination of Partial Molar quantities.
 - (3) Discuss applications of phase rule to one or three component system.
- (b) Answer any **one** of the following : 4
- (1) The molar volume of pure methanol is 40 cc/mole. Also the volume of a solution containing 1000 gram of water and 'n' moles of methanol is given by

$$V = 1000 + 35n + 0.5 n^2$$
 Calculate the partial molar volume for methanol for molality, $m = 0$ and for $m = 1$.
 - (2) H_2 gas at $1000^\circ C$ and 300 atm pressure occupies a volume of $0.1191 \text{ dm}^3/\text{mole}$. When the values of α are plotted Vs, pressure, the area under the curve is found to be $4.92 \text{ atm dm}^3/\text{mole}^{-1}$. Calculate the departure from ideal behaviour, α , the fugacity f , and the activity coefficient for H_2 at $100^\circ C$ and 300 atm pressure.

- 4 (a) Answer any **two** of the following : 10
- (1) What is partition function ? Derive an equation for rotational partition function.
 - (2) Discuss most probable distribution.
 - (3) Explain entropy production in irreversible thermodynamics.
- (b) Answer any **one** of the following : 4
- (1) Calculate the rotational partition function for NH_3 at 27°C .
 The three moment of inertia are :
 $I_A = I_B = 2.78 \times 10^{-47}$ and
 $K = 1.38 \times 10^{-23} \text{ JK}^{-1}$
 $h = 6.62 \times 10^{-34} \text{ Js}$. $I_C = 4.33 \times 10^{-47} \text{ kg}$.
 σ for $\text{NH}_3 = 3$
 - (2) Explain : Grand Canonical and Micro-canonical ensembles.
- 5 Answer any **seven** of the following : 14
- (1) Define harmonic oscillator.
 - (2) Calculate the ionic strengths of solutions that contain
 - (a) 0.3 M CaCl_2
 - (b) 0.1 M Na_2SO_4 + 0.2 M NaCl
 - (3) What is meant by activity ? How it is related to pressure and fugacity ?
 - (4) Give the limitations of phase rule.
 - (5) Give applications of Extended Huckel Theory.
 - (6) Definition of Freedom (degree) in phase rule.
 - (7) By using Stirling approximation calculate $\ln N$, where N_A is the Avogadro's number.
 - (8) Application of Extended Huckel theory.
 - (9) Explain the terms variation theory.
 - (10) Give the limitations of the first law of thermodynamics.