



**KP-1639**

Seat No. \_\_\_\_\_

**M. Sc. (Sem. I) Examination**

**November/December – 2017**

**CHN-403 : Physical Chemistry : Paper-III**

Time : 3 Hours]

[Total Marks : 70

- Instructions :**
- (1) Each question carries 14 marks.
  - (2) Figures to the right indicates marks of the question.

- 1 (a) Answer the following : (any two) 10
- (1) Describe briefly the various postulates of wave mechanics.
  - (2) Set up and solve the Schrodinger wave equation for : one-dimensional simple harmonic oscillator.
  - (3) Mention the perturbation theory.
- (b) Answer the following : (any one) 14
- (1) Discuss : Variation theorem.
  - (2) Short note about "The rigid rotor".

- 2 (a) Answer the following : (any two) 10
- (1) Discuss the eigen functions for angular momentum.
  - (2) Short note on "Russell-Saunders terms and coupling schemes".
  - (3) Write a note on Huckel theory of conjugated systems.
- (b) Answer the following : (any one) 4
- (i) Explain : Pauli exclusion principle.
  - (ii) Apply the Huckel-Molecular orbital theory to the following :
    - (1) Ethylene
    - (2) 1, 3 - Butadiene.
- 3 (a) Answer the following : (any two) 10
- (i) Explain the term partial molar free energy. "Derive the Gibbs-Duhem equation".
  - (ii) Define fugacity : Discuss the methods used to determine its value.
  - (iii) Discuss about "EMF method" for determine of activity and activity coefficient.
- (b) Answer the following : (any one) 4
- (i) From the plot of  $\alpha$  Vs P for CO, the area under the curve between 0 and 100 atm pressure was found to be  $0.0875 \text{ atm}^2$ . Calculate the fugacity of CO at 100 atm and  $0^\circ\text{C}$ .

- (ii) Calculate the volume of an ideal solution at 25°C that contains exactly 10 mole of ethanol and 6 mole of water. The molar volumes of ethanol and water being 58.7 cm<sup>3</sup> and 18.1 cm<sup>3</sup> respectively. If the partial molar volumes of ethanol water are 57.6 and 16.5 cm<sup>3</sup> respectively, what would be the change in volume when 10 mol of ethanol is mixed with 6 mole of water ?

4 (a) Answer the following : (any two) 10

- (i) Give an account of Thermodynamics probability.
- (ii) What is partition function ? Derive an equation for rotational partition function.
- (iii) Mention and prove Prigogine's principle of minimum entropy production.

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

- (i) Calculate the rotational partition function for hydrogen molecule at 300°k. Moment of inertia of hydrogen molecule is  $4.59 \times 10^{-4} \text{ kg.m}^2$ , symmetry number = 2.
- (ii) Explain : grand canonical and micro-canonical ensembles.

5 Attempt any seven of the following :

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- (i) Define : Laplacian operator.
- (ii) What are electron spin and antisymmetry ?
- (iii) Explain : electron density.
- (iv) Explain entropy. What are its units ?
- (v) Calculate the ionic strength of the following solutions :  
(1) 0.1M  $\text{BaCl}_2$  (2) 0.1M  $\text{Na}_3\text{PO}_4$
- (vi) Define the term phase and degree of freedom with examples.
- (vii) What is meant by activity ? How it is related to pressure and fugacity ?
- (viii) Any one sentence of "Second law of thermodynamics."
- (ix) Define the term probability.
- (x) Using stirling approximation and the value of  $6!$ . Compare this value without stirling approximation, comment on the result.