



KK-5917

Seat No. _____

M.Sc. (Sem. I) Examination

November / December - 2014

CHN - 403 (P) : Physical Chemistry

Time : 3 Hours]

[Total Marks : 70

- Instructions:** (1) Attempt all questions
(2) All questions carry equal marks.

1. (A) Write any 02 of the following **02x4=08**
- Explain Schrodinger's wave equation by deriving an equation..
 - Discuss the applications of variation method taking the example of multi electron system.
 - Explain concept of harmonic oscillator in wave mechanics.
 - Calculate the spacing between energy levels for an electron of mass 10^{-30} Kg in one dimensional box of 1.0 \AA length.
- (B) Do any two of the following. **02x3=06**
- Derive an equation for wave function and energy of the particles in one dimensional box.
 - Use principle of minimization energy and apply perturbation treatment to Helium atom.
 - Discuss postulates of quantum mechanics.
 - What is the wavelength of the light absorbed when an electron in a linear molecule 10 \AA long makes a transition from energy level, $n=1$ to level $n=2$.

2. (A) Answer any two of the following 02x3=06
- i. Discuss Slater- Condon parameters.
 - ii. Explain Eigenfunctions and Eigenvalues for angular momentum operator.
 - iii. Derive term separation energies of the p^n configuration.
 - iv. Explain the concept of atomic states, atomic terms and term symbols.
- (B) Attempt any two of the following 02x4=08
- i. Write a note on Huckel's theory of conjugated systems.
 - ii. Explain the concept of ordinary and generalised angular momentum.
 - iii. Discuss term separation energies for the d^n configurations.
 - iv. Show that total angular momentum and its z-component cannot be specified simultaneously.
3. (A) Do any two of the following 02x3=06
- i. Define phase rule and apply it to three component system.
 - ii. The molar volume of pure methanol is 40cc/mole. Also the volume of solution containing 1000 g of water and n moles of methanol is given by $V=1500 + 40n + 0.5n^2$
Calculate the partial molar volume for methanol for molality, $m=0$ and for $m= 1$.
 - iii. Define activity and determine the activity coefficient of electrolytes using E. M. F. method.
 - iv. Define third law of thermodynamics as principle of unattainability and determine entropy of solids.
- (B) Attempt any two of the followings 02x4=08
- i. Define partial molar properties and determine partial molar volume using density measurement method.

- ii. Derive an equation for activity coefficients of electrolytes using Gibb's Duhem concept.
- iii. Vapour pressure of a pure liquid is 100 torr at 25°C while its pour pressure from 95 % solution at the same temperature is only 90 torr. What is the activity of the liquid in the solution? What is the activity coefficient for it?
- iv. Write note on
(a) Chemical potential (b) Molar Enthalpy
4. (A) Answer any two of the followings. **02x3=06**
- i. Derive an equation for statistical equilibrium observed in systems.
- ii. Explain the relation between partition function and thermodynamic parameter as free energy.
- iii. Define phenomenological equations used in non equilibrium thermodynamics.
- iv. Calculate the mean vibrational energy of Iodine vapours at 298 K. The vibrational levels above the zero point energy are 213.3, 425.39, 845.93 and 1045.38 cm^{-1} . Partition function for Iodine is given as 1.55.
- (B) Do any two of the followings. **02x4=08**
- i. Derive an equation showing Internal Energy in terms of partition function.
- ii. Discuss the concept of entropy production in the irreversible processes.
- iii. Discuss thermodynamic probability.
- iv. Calculate the translational energy (1,1,2) for an oxygen molecule in a container of the side $a=0.1\text{m}$. Express the results in S. I. units.

5. Attempt 07 from the following

02x7=14

- I. First law
 - II. Molar Heat content
 - III. Activity of electrolytes
 - IV. Kinetic energy operator
 - V. Conditions for acceptable wave
 - VI. Angular momentum operator
 - VII. Russel- Saundes terms
 - VIII. Assembly and ensamble
 - IX. Generalised fluxes
 - X. Microstate and Macrostate
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