PG – 551

I Semester M.Sc. Examination, January 2017
(CBCS)
CHEMISTRY
C-103 : Physical Chemistry – I

Time : 3 Hours | Max. Marks : 70

Instruction *: Answer Question No.* ***1*** *and* ***any five*** *of the remaining questions.*

1. Answer **any ten** of the following : **(2×10=20)**

   a) Write the concepts of linear and Hermition operators.

   b) What are eigenfunctions and eigenvalues ?

   c) Determine the degeneracy and energy levels for the particle in a 3D box having an energy $18h^2/8ma^2$.

   d) Write about slater determinants.

   e) What is Zeeman effect ?

   f) State and prove variation theorem.

   g) Mention the limitations of collision theory.

   h) Define the terms 'chain length' and 'chain inhibition'.

   i) Write the reaction mechanism for the pyrolysis of acetaldehyde and mention the active reactive species.

   j) Explain Lock and Key theory of enzyme catalysis.

   k) List out the limitations of Lindemann's theory of unimolecular reactions.

   l) Arrive and explain Laplace equation for pressure difference across curved surface.

2. a) Set up and solve time dependent Schrodinger wave equation.

   b) Apply Schrodinger equation for one dimensional simple harmonic oscillator.

(5+5=10)

P.T.O.

3. a) Give the operators for x, y and z components of angular momentum.

   b) Brief Ladder operator. Evaluate $\left[\hat{L}_+, \hat{L}_z\right]$.

   c) Represent the total wave functions for the 1s, 2p and 3s orbitals of hydrogen atom. **(3+3+4=10)**

4. a) Formulate the Schrodinger equation for the hydrogen atom in spherical polar co-ordinates and separate it into ϕ, θ and R equations.

   b) Define spin-orbital coupling. Explain the origin of doublet in Na atomic spectra.

   c) What are radial angular distribution functions ? Point out their significance. **(4+3+3=10)**

5. a) Apply Schrodinger perturbation theory to electron in a box and find its solution.

   b) Obtain the rate expression for predicting the influence of primary salt effect on the reaction rates. **(5+5=10)**

6. a) Discuss the kinetics and mechanism of photochemical reaction between H_2 and Br_2.

   b) Describe the stopped flow technique for the study of fast reactions. **(5+5=10)**

7. a) Using Lineweaver-Burk equation, explain the effects of inhibitors on enzyme activity.

   b) Explain the influence of pH on enzyme activity.

   c) The rate constant for a first-order reaction is 6.0×10^{-5} sec^{-1} at 298K and 10.5×10^{-4} sec^{-1} at 318K. Calculate the energy of activation for this reaction. **(4+3+3=10)**

8. a) Derive the Gibb's adsorption equation.

   b) Depict and explain the types of adsorption isotherms.

   c) Explain the relaxation time of a chemical transformation in the study of fast reactions. **(4+3+3=10)**