I Semester M.Sc. Examination, January/February 2018 (CBCS Scheme) CHEMISTRY C - 103: Physical Chemistry - I

Time: 3 Hours

: 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) What are operators ? Explain Hamiltonian operator.
- b) Mention the significance of quantum mechanical tunneling phenomenon.
- c) Provide an explanation for the terms normalization and orthogonality of wave functions.
- d) Write about Slater determinants.
- e) Explain term symbol with an example.
- f) Justify the need for approximation methods in quantum mechanics.
- g) Give a comparative account of collision and transition state theories.
- h) State and explain steady state kinetics.
- i) What is temperature coefficient? How it can be evaluated?
- j) When water is subjected to the temperature jump method, the relaxation time for the return to the equilibrium at 30° is 40 × 10⁻⁶s. Calculate the rate constants for the forward and reverse reaction.
- k) Explain the effect of temperature on enzyme activity.
- I) Comment on mechanical adsorption.
- 2. a) Formulate time-independent Schrodinger wave equation.
 - b) Give the physical significance of wave function.
 - State and explain any three postulates of quantum mechanics. (4+3+3=10)
- a) Apply Schrodinger equation for a rigid rotator and obtain its normalized eigen functions and eigen values.
 - b) Outline the total wave functions of hydrogen atom.
 - c) Give a brief account of radial and angular wave functions diagrams. (4+3+3=10)



- a) Obtain expressions for first order corrections in energy and wave function for a non-degenerate system according to Rayleigh Schrödinger Perturbation theory.
 - b) Demonstrate the Stern-Gerlach experiment.

(6+4=10)

- 5. a) Give the operators for x, y and z components of angular momentum.
 - Explain primary and secondary salt effects. Predict the influence of increasing ionic strength of the medium on the rate of following reactions;
 - I) CO (NH₃)₅ Br²⁺ + NO₂ → products
 - ii) $S_2O_8^2 + I^- \rightarrow \text{products}$
 - iii) CH₃COOC₂H₅ + OH⁻ → products.

(5+5=10)

- a) Discuss the kinetics and mechanism of thermal chain reaction between H₂ and Br₂.
 - b) Outline the shock tube technique for the study of ast reactions.

(6+4=10)

- a) Derive Michaelis-Menten equation for a single substrate enzyme catalyzed reaction using steady state approximation.
 - b) Discuss the kinetics and mechanism of unimolecular reactions as proposed by Lindemann.
- a) Obtain Kelvin equation for variour pressure droplets and mention its significance.
 - Explain the use of BET equation in the determination of surface area of a solid
 - c) Write a brief account of catalytic activity of surfaces.

(4+3+3=10)