**SEMESTER-I**
**Paper-S-1043**
**Physical Chemistry**

**Time: 3 Hrs.** **M.M. 75 marks**

**Note: The paper will be divided into two sections.**

Section-A One question with 10 parts (short answer word limit 20) spread over whole syllabus. Each part will be of 1 mark and candidate is required to attempt all the ten parts

**Total 10 marks**

Section-B Five questions (answer not exceeding 500 words) are from each Unit with internal choice will be asked and the candidate is required to attempt all five questions. Each question will be of 13 marks

**Total 65 marks**

**ESSENTIAL –All students must have knowledge of these topics of mathematics-**

Differentiation and Integration of some simple terms, Differential equations, partial differential equations, series solutions and special functions, linear vector spaces, transformation of coordinate matrix, representation of operators, eigenvalue problem, orthonormal sets, Fourier and Laplace transforms.

**UNIT-I**

**Quantum chemistry:** The Schrodinger equation and the postulates of quantum mechanics, solutions of the Schrodinger equation to some model system viz.. particle in a box, the harmonic oscillator.

**Approximate methods:** First order time-independent perturbation theory for non-degenerate states. Variation theorem and variational methods. Use of these methods illustrated with some examples (particle in a box with a finite barrier, anharmonic oscillator, approximate functions for particle in a box and hydrogen atom).

**UNIT-II**

**Angular momentum**: Ordinary angular momentum, generalized angular momentum, eigen functions and eigen values of angular momentum, operators, algebra of operators, ladder operators, addition of angular momenta, spin, antisymmetry and Pauli's exclusion principle.

**Electronic structure of atoms:** Electronic configuration, Russell-Saunder's terms coupling schemes, molecular orbital theory, Huckel theory of conjugated systems, bond order and charge density calculations, application to ethylene and butadiene.

**UNIT-III**

**Chemical dynamics:** Methods of determining rate laws and mechanism, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and thermodynamic parameters, ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, general features of fast reactions.

**UNIT IV**

Homogeneous catalysis, kinetics of enzyme reactions, chain reactions, photochemical reactions (Hydrogen-bromine and hydrogen-chlorine reactions) oscillatory reactions (Belousov-Zhabotinsky reaction),

## UNIT V

**Macromolecules:** Definition, types of polymers, electrically conducting, fire resistant and liquid crystal polymers, kinetics of polymerization, mechanism of polymerization, molecular mass, number and mass average molecular mass, molecular mass determination (osmometry, viscometry, diffusion and light scattering methods,GPC), sedimentation.

**Recommended Texts:**


1. Lowe, J. P. & Peterson, K. Quantum Chemistry Academic Press (2005).
2. McQuarrie, D. A. Quantum Chemistry Viva Books Pvt. Ltd.: New Delhi (2003).
3. Mortimer, R. G. Mathematics for Physical Chemistry 2nd Ed. Elsevier (2005).
4. Pilar, F. L. Elementary Quantum Chemistry 2nd Ed., Dover Publication Inc.: N.Y. (2001).
5. Atkins, P. W. & Paula, J. de Atkin's Physical Chemistry 8th Ed., Oxford University Press(2006).
6. Levine, I. L Quantum Chemistry 5th Ed., Prentice-Hall Inc.: New Jersey (2000).
7. Engel, T. & Reid, P. Physical Chemistry Benjamin-Cummings (2005).
8. McQuarrie, D. A. & Simon, J. D. Physical Chemistry: A Molecular Approach 3rd Ed., Univ. Science Books (2001).
9. Chemical Kinetics, K.J. Laidler, Mcgraw-Hill
10. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose, McMillan.