CHEM.C-12 (T): PHYSICAL CHEMISTRY-V: QUANTUM CHEMISTRY & SPECTROSCOPY

Total Marks:100 **(Credits:03)**

UNIT–I: Quantum Chemistry-I

Quantum mechanical operators, Postulates of quantum mechanics, Schrödinger equation and its application to free particle and "particle-in-a-box" (rigorous treatment), quantization of energy levels, zero-point energy and Heisenberg Uncertainty principle; wave functions.
Qualitative treatment of the simple harmonic oscillator model of vibrational motion: Setting up of the Schrödinger equation and discussion of solution and wave functions. Vibrational energy of diatomic molecules and zero-point energy.

UNIT–II: Quantum Chemistry-II

Qualitative treatment of hydrogen atom and hydrogen-like ions: setting up of Schrödinger equation in spherical polar coordinates, radial part, and quantization of energy (only final energy expression).
Chemical bonding: Covalent bonding, valence bond and molecular orbital approaches, Born-Oppenheimer approximation, LCAO-MO treatment of H^+. Bonding and antibonding orbitals. Qualitative extension to H_2. Comparison of LCAO-MO and VB treatments of H_2 (only wave functions, detailed solution not required) and their limitations.

UNIT–III: Molecular Spectroscopy

Interaction of electromagnetic radiation with molecules and various types of spectra;
Rotation spectroscopy: Selection rules, intensities of spectral lines, determination of bond lengths of diatomic and linear triatomic molecules, isotopic substitution.
Vibrational spectroscopy: Classical equation of vibration, computation of force constant, amplitude of diatomic molecular vibrations, anharmonicity, Morse potential, dissociation energies, fundamental frequencies, degrees of freedom for polyatomic molecules, modes of vibration.
Electronic spectroscopy: Franck-Condon principle, electronic transitions, singlet and triplet states, fluorescence and phosphorescence, dissociation and predissociation.

UNIT–IV: Photochemistry

Characteristics of electromagnetic radiation, Lambert-Beer's law and its limitations, physical significance of absorption coefficients. Laws of photochemistry, quantum yield, examples of low and high quantum yields, photochemical equilibrium and the differential rate of photochemical reactions, photosensitized reactions, quenching.

ReferenceBooks:

1. Banwell,C.N.&McCash,E.M.*Fundamentals of Molecular Spectroscopy* 4th Ed.Tata McGraw-Hill: New Delhi (2006).
2. Chandra,A.K.*Introductory Quantum Chemistry* TataMcGraw-Hill (2001).
3. House, J.E. *Fundamentals of Quantum Chemistry* 2nd Ed. Elsevier: USA(2004).
4. Kakkar,R.*Atomic&Molecular Spectroscopy*: *Concepts & Applications*, Cambridge University Press (2015).
5. Lowe, J.P. & Peterson, K. *Quantum Chemistry*, Academic Press (2005).