CHEMISTRY
(Major)
(5th Semester)
Course No.: **CHM-DSC-301**
Quantum and Photochemistry
Contact Hours: 60; Credits: 04
Full Marks = 100[End Semester Exam (70) Internal Assessment (30)]
Pass Marks = 40 [End Semester Exam (28) Internal Assessment(12)]

Unit-1: Quantum Chemistry-I

Introduction to black-body radiation and distribution of energy, photo-electic effect, concept of quantization, wave particle duality (de-Broglie's hypothesis), The uncertainty principle, The wave function: wave function and its interpretation, conditions of normalization and Orthogonality and its significance. Basic idea about operators, Eigen function and values, Postulates of quantum mechanics. Schrodinger equation and application to free-particle and particle in a box, boundary conditions. Extension to two dimensional and three dimensional box wave functions and energies, degeneracy.

Unit-2: Quantum Chemistry-II

Quantitative treatment of simple harmonic oscillator model, setting up of Schrodinger equation and discussion of solution of wave functions. Vibrational energy of diatomic molecules and significance of zero point energy. Rigid rotator model and discussion of application of Schrodinger equation.

Unit-3: Chemical Bonding

Variation theorem, Valence bond and molecular orbital approaches, LCAO-MO treatment of H_2, H_2^+; bonding and anti-bonding orbitals, Comparison of LCAO-MO and VB treatments of H_2 (only wave functions, detailed solution not required) and their limitations. Spin state of two electron system, Singlet and triplet state. Setting up of Schrödinger equation for many-electron atoms (He, Li), Qualitative description of LCAO-MO treatment of homonuclear and heteronuclear diatomic molecules (HF, LiH), calculation of Bond order.

Unit-4: Hybridization and Shape

Quantum mechanical approach of SP^3, SP^2 and SP hybridization and bond angle. The pi-electron approximation, the Huckel MO approximation. Simple Huckel treatment of ethane, allyl and butadiene system. Huckel's rule of aromaticity, delocalization energy of cyclic system.

Unit-5: Photochemistry

Difference between thermal and photochemical process, Laws of photochemistry: Grothus-Drappers law, Stark-Einstein Law, Jablonski diagram depicting various processes occurring in the excited states, qualitative description of fluorescence, phosphorescence, non-radiative processes of internal conversion, intersystem crossing, quantum yield, example of high and

low quantum yield reaction, Photosensitized reaction, quenching, Chemiluminescence. Kinetics of photochemical reactions ($H_2 + Br_2 \rightleftharpoons HBr$, $2HI \rightleftharpoons H_2 + I_2$),

Reference Books:

- K. Chandra, Introductory Quantum Chemistry Tata McGraw-Hill
- B.K Sen , Quantum Chemistry including Spectroscopy 3rd edition, Kalyani Publishers.
- J. P. Lowe, & K. Peterson, Quantum Chemistry, Academic Press (2005).
- J. E House, Fundamentals of Quantum Chemistry 2nd Ed. Elsevier: USA.
- D. A., Macqurre, Quantum Chemistry.
- Peter W. Atkins, and Friedman, S. Ronald, Molecular Quantum Mechanics 5th Edition.
- R. Kakkar, Atomic & Molecular Spectroscopy, Cambridge University Press