

**Module-I****(12 hours)**

**Quantum Chemistry-I:** Operators in Quantum mechanics: Linear, Hermitian and Angular Momentum operators, Eigenvalue problem.

Basic postulates of quantum mechanics. The Schrodinger equation, Particle in 1,2 and 3-dimensional boxes, degeneracy.

**Module-II****(8 hours)**

**Quantum Chemistry-II:** Harmonic oscillator, Spherical Coordinates: Rigid rotator, Solution of the Schrodinger equation for Hydrogen like atoms, Significance of n, l and m quantum numbers. Linear Variation and Perturbation Methods. Multielectron atoms, spin quantum number, Ground and excited state of helium atom.

**Module-III****(10hours)**

**Quantum Chemistry-III:** Hydrogen Molecule ion, Born-Oppenheimer approximation, LCAO-MO approximation, Hydrogen Molecule, Valence Bond and Molecular Orbital Theory. Homonuclear and heteronuclear diatomic molecules (HF, CO, NO)

**Module-IV****(10 hours)**

**Group Theory:** Symmetry Elements and Symmetry Operations, Point Groups, Representation of Groups, Reducible and Irreducible Representation; Character Tables, Applications of Great Orthogonality Theorem.

**Text Books (Quantum Chemistry and Group Theory)**

1. D. A. McQuarrie and J. D. Simon, Physical Chemistry: A Molecular Approach, Viva Student Edition, 2015.
2. D. A. McQuarrie, Quantum Chemistry, Viva Student Edition, 2015.
3. M. S. Gopinathan and V. Ramakrishnan, Group Theory in Chemistry, Vishal Publishers, 1988.
4. Cotton, F. A. Chemical Applications of Group Theory, 3<sup>rd</sup> Edn., John Wiley and Sons, 2003.

**Reference Books**

1. N. Levine, 'Quantum Chemistry', 4th Edn., Prentice Hall India, 2001.
2. A. K. Chandra, Introductory Quantum Chemistry, Tata McGraw Hill, 1994.
3. Jack Simons, Introduction to Theoretical Chemistry, Cambridge University Press, 2003.
4. P. W. Atkins. Molecular Quantum Mechanics, Oxford University Press (1986).