UNIT – I Basic Principles of Quantum Mechanics

a) Mathematical Concepts.

Coordinate system: Cartesian, cylindrical polar and spherical polar coordinates and their relationships. Complex numbers: Definition, complex conjugate, absolute value of a complex number, complex functions.

Elements of operator algebra: Definition of an operator, Linear and nonlinear operators, ‘Del’ and del squared’ operators and their expression in cylindrical and spherical polar coordinates. Eigen functions and Eigen values of an operator, Eigen value equation, Hermitian operators, Eigen functions of commuting operators, well-behaved functions, normalized and orthogonal functions.

b) Brief history of quantum mechanics

Plank’s quantum postulates, Eienstein’s quantum theory of radiation, Explanation of photo electric effect, Milliken’s verification of Einstein’s photoelectric equation, wave-particle duality of radiation, wave particle duality of particles, de Broglie matter waves, Electron diffraction, Heisenberg’s Matrix Mechanics (brief mention), Schrödinger’s wave mechanics, Deduction of Schrödinger equation from classical wave equation.

c) Formulation of quantum mechanics

The Postulates of quantum mechanics, State functions postulate, Operator postulate, Eigen value postulate, Expectation value postulate, Postulate of time dependent Schrodinger Equation of motion, Conservative system and time- independent Schrodinger equation, Stationary states, Formulation of a quantum mechanical problems.

UNIT – II Quantum mechanics of translational, vibrational and rotational motions

a) Translations Motions

The particle in a one-dimentional box –complete treatment. The particle in a three-dimentional box (consider rectangular and cubic boxes), Separation of variables, Degeneracy, Symmetry breaking, Treatment of more than one particle (non-interacting) in a box. Introduction to Tunneling.

b) Vibrational motion

Harmonic oscillator (complete treatment): Method of power series, Hermite equation and Hermite polynomials, Recursion formula, Rodrigue’s formula, Wave functions and energies, Important features of the problem, Harmonic oscillator and molecular vibrations, Three dimensional harmonic oscillator.
c) **Rotational motion**
Rigid rotator (complete treatment): The wave equation in spherical polar coordinates. Planar rigid rotator (or Particle on a ring), The Phi- equation, Solution of the Phi-equation, Handling of Imaginary wave functions, Wave functions in the real form, Polar diagrams. 
Nonplanar rigid rotator (or particle on a sphere), Separation of variables. The Phi-equation and the Theta-equation and their solutions, Legendre and Associated Legendre equations, polynomials, Spherical harmonics (Imaginary and real forms). Polar diagrams of spherical harmonics. Spherical harmonics as eigen function of angular momentum operators $L^2$ and $L_z$. Quantization of angular momentum, Angular momentum quantum numbers, Space quantization.

**UNIT- III Quantum Mechanics of atoms**

a) **Hydrogen – Like atoms**

b) **Many-electron atoms and approximations methods**
Hartree-Fock Self-Consistent Field (HG-SCF) method. Slater’s treatment of complex atoms, Slater Orbitals, Slater’s rules, Slater orbitals.

c) **Electron spin and atomic structure**
Symmetric and antisymmetric wave functions, Slater determinants, Pauli’s exclusion principle.
Vector model of atoms and spectroscopic terms. Coupling of angular momenta, LS and jj-couplings, LS coupling and Sepctroscopic term symbols for atoms, Brief mention of selection rule in atomic spectroscopy.

**UNIT IV- Molecular symmetry and Group Theory**
Fundamental concepts – Symmetry operations and elements, symmetry point groups and classification.
Representation of groups- Irreducible and reducible representations, Great orthogonality theorem, construction of Character Tables ($C_{2v}$, $C_{3v}$, $C_{2h}$, $C_{4v}$).
Connection between group theory and quantum mechanics. MO treatment of molecules using group theory- SALC combination, construction of MOs. Application of group theory to molecular vibrations - Vibrational mode and their symmetric, selection rules for Raman and IR activity and their determination

**Text Book/Reference**

1. Modern Physics, A Beiser, S. Mahajan and S. Raj Chouthury
2. Modern Quantum Mechanics, J.J. Sakurai
3. Quantum Mechanics G. Arwdhar
4. Modern Approach to Quantum Mechanics J.S. Townsent
5. Chemical Applications of Group Theory by F.A. cotton