In.M.Sc, Applied Chemistry (5 years)

6th Semester

FCYC603	Quantum Theory	3-1-0	4

Module-I

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

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

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

Selected Text / Reference Books:

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, 3rd Edn., John Wiley and Sons, 2003.
5. N. Levine, 'Quantum Chemistry', 4th Edn., Prentice Hall India, 2001.
6. A. K. Chandra, Introductory Quantum Chemistry, Tata McGraw Hill, 1994.
7. Jack Simons, Introduction to Theoretical Chemistry, Cambridge University Press, 2003.
8. P. W. Atkins. Molecular Quantum Mechanics, Oxford University Press (1986).