

Course Code	Course Name	Credits
26CH511	QUANTUM CHEMISTRY AND GROUP THEORY	04

Course Objectives

- To understand the fundamental principles of quantum mechanics and their application to atomic and molecular systems.
- To apply quantum mechanical models and theories to explain molecular structure and bonding.
- To analyze molecular symmetry using group theory and apply it to chemical systems.

Learning Outcomes

Upon successful completion of this course it is intended that a student will be able to:

- Understand the fundamentals of quantum mechanics, including wave-particle duality, Schrödinger equation, and operator concepts.
- Apply quantum mechanical models such as particle in a box, harmonic oscillator, and rigid rotor to molecular systems.
- Analyze chemical bonding using VB, MO, and Hückel theories, including hybridization and approximations.
- Apply group theory concepts to determine molecular symmetry, point groups, and construct character tables.

Unit 1 - Quantum chemistry-I (10 Hrs.)

Inadequacy of Classical Mechanics; Black Body Radiation; Planck's Quantum Concept; Photoelectric Effect; Bohr's Theory of Hydrogen Atom; Hydrogen Spectrum; Wave-Particle Dualism; Uncertainty Principle; Decline of Old Quantum Theory; Schrödinger Equation; Postulates of Quantum Mechanics; Operator Algebra (Linear Operators, Hermitian Operators, Eigenfunctions and Eigenvalues, Angular Momentum Operator); Commutation Relations and Related Theorems.

Unit 2 – Quantum chemistry-II (15 Hrs.)

Normalization of the Wave Function; Orthogonality of the Particle in a One-Dimensional Box Wave Function; Illustration of the Uncertainty Principle and the Principle of Correspondence (Particle in a One-Dimensional Box); Particle in a Three-Dimensional Box; Separation of Variables; Solution of the Schrödinger Equation for the One-Dimensional Harmonic Oscillator; Harmonic Oscillator Model of a Diatomic Molecule; Illustration of the Uncertainty Principle and the Principle of Correspondence (Harmonic Oscillator); Solution of the Schrödinger Equation for a Rigid Rotor; Rigid Rotor Model of a Diatomic Molecule.

Unit 3 - Quantum chemistry-III (10 Hrs.)

Born-Oppenheimer Approximation; Valence Bond (VB) Theory of Hydrogen Molecule; Molecular Orbital (MO) Theory of Hydrogen Molecular Ion (H_2^+); Coulomb Integral; Exchange Integral; Overlap Integral; Calculation of Energy and Overlap Integrals; Hybridization (sp , sp^2 , sp^3 Orbitals); Hückel Molecular Orbital Theory; Applications of Hückel Theory (Ethylene, Butadiene, Benzene, Cyclobutadiene, Trimethylamine, Bicyclobutadiene, Allyl Systems); Hartree-Fock Method; Self-Consistent Field (SCF) Method; Roothaan Equations.

Unit 4 – Group theory-I (12 Hrs.)

Symmetry Elements and Symmetry Operations; Identical and Equivalent Configurations; Rotation Axis of Symmetry; Reflection Symmetry Planes; Inversion Center; Improper Rotation Axis (Rotation-Reflection); Successive Symmetry Operations (Commutative and Non-Commutative); Inverse Operations; Definition of a Group; Basic Properties of a Group; Abelian Groups; Isomorphic Groups; Similarity Transformation and Classes; Group Multiplication Tables; Symmetry Classification of Molecules into Point Groups (Schoenflies Symbols); Difference between Point Group and Space Group.

Unit 5 - Group theory-II (13 Hrs.)

Matrix Representation of Symmetry Operations and Point Groups; Reducible and Irreducible Representations; The Great Orthogonality Theorem; Construction of Character Tables; Direct Product; Projection Operators; Symmetry of Hybrid Orbitals; Determination of Characters for Irreducible Representations of C_{2v} and C_{3v} Point Groups (Using Orthogonality Theorem).

Reference Books:

- K. Raman, Group Theory and its Application to Chemistry, 1990, Tata McGraw-Hill, New Delhi.
- S. Glasstone and D. Lewis, Elements of Physical Chemistry, Mac Millan & Co Ltd., London.
- P.W. Atkins, Physical Chemistry, 5th Edn., 1994, Oxford University press.
- M.V. Sangaranarayanan, V. Mahadevan, Text Book of Physical Chemistry, 2nd Edn., 2011, Hyderabad, Universities Press, India.

Websites and eLearning Sources:

- <https://nptel.ac.in/courses/104106128>
- <https://nptel.ac.in/courses/103101568>
- <https://www.youtube.com/watch?v=1NHraQQMbA&list=PLgqUj5LKfMKhLkpr1q8C1wWcsZuARrF8d>

COs and Bloom's Taxonomy Mapping – 26CH511		
Course Outcomes	On completing P.G. program the students will be able to	BTL
CO1	Students should be able to solve the Schrödinger equation for various systems and interpret the physical meaning of wave functions.	K1, K2
CO2	Apply group theory to determine which molecular orbitals are bonding, non-bonding, or antibonding based on symmetry considerations.	K3
CO3	Analyze selection rules derived from group theory to predict which electronic transitions are allowed or forbidden in spectroscopy.	K4
CO4	Evaluate theoretical models and computational simulations to solve complex chemical problems.	K5
CO5	Develop skills to analyze experimental data in light of quantum chemical and symmetry principles.	K6

BTL K1 and K2 – remembering and understanding, K3- Applying, K4 – Analyse, K5- Evaluate and K6- Create

Relationship Matrix – 26CH511												
Course Outcomes	Programme Outcomes (POs)						Programme Specific Outcomes (PSOs)					Mean Score of Cos
	PO1	PO2	PO3	PO4	PO5	PO6	PSO1	PSO2	PSO3	PSO4	PSO5	
CO1	1	2	2	3	2	2	3	3	3	2	1	2.18
CO2	1	2	2	2	1	2	1	1	3	3	1	1.72
CO3	1	2	2	1	3	1	2	3	1	2	2	1.81
CO4	2	1	3	3	2	3	1	2	2	2	1	2
CO5	1	2	1	2	3	2	1	1	3	3	3	2
Total											1.94	

Mean Score: 3- High, 2- Medium/Moderate, 1-Low

