

FCYE505	Symmetry and Group Theory	3-1-0	3
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Module I

Basic Group theory , Molecular symmetry, Symmetry Groups

Algebraic Systems – Common properties of Operators – Levels of Abstraction – Subsystems – Direct Products – Isomorphisms - Axioms and theories of group – Abelian and cyclic groups – Finite subgroups and Homomorphisms - Similarity Transformation and Classes - Cosets and Permutation Groups.

Symmetry Elements and operations – Planes – Axes - Inversions – Improper Axes – Products of Symmetry Operations – Equivalence symmetry elements and operations – Relations between symmetry operations – Classes – Symmetry groups with multiple higher order axes – Symmetry Point groups – Matrix representation of symmetry operations

Module II

Group Theory in Molecular Quantum Chemistry

Representation of groups - Character - Reducible and Irreducible Representations - Great Orthogonality Theorem - Construction of Character Tables – Cyclic groups - Double groups - Direct Products – Complete and Incomplete Projection Operators – Constructions of Symmetry adapted Linear Combinations.

Module III

Applications

Symmetry properties of Hamiltonian operator - Wave functions as basis for Irreducible Representations - Transition moment integrals - selection rule for spectral transitions - Mutual exclusion principle – LCAO – MO Approximation – Symmetry factoring of secular equations-Ligand field theory – Molecular Vibrations – Woodward-Hoffmann Cyclization rules.

Selected Text/Reference Books:

1. F. A. Cotton: Chemical Applications of Group Theory, Wiley Eastern, 1985.

Further Reading:

2. A. M. Lesk, Introduction to symmetry and group theory for chemists, Kluwer, NY, 2004.

3. A. Vincent, Molecular Symmetry and Group theory, A Programmed Introduction to chemical applications, Wiley, New York, 2001.

4. R. L. Carter, Molecular Symmetry and Group theory, Wiley, NY, 1997.

5. R. B. Woodward and R. Hoffmann, Conservation of Orbital symmetry, Verlag Chemie GmbH, NY, 1970.

6. Symmetry and Spectroscopy of Molecules, 2nd Edition, K. V. Reddy, New Age International Publishers