

Course Title: Group Theory in Chemistry

Semester: VII

Course Code: CH-454

Credit Hours: 3-0

Pre-requisite: Nil

1. Course Objectives. Students will acquire knowledge about symmetry; operations & elements, point groups, character tables and applications of group theory.

2. Course Outcomes. At the end of the course, students will be able to understand the symmetry; operations & elements, point groups, development of character tables for various point groups and applications of group theory.

3. Course Outline

Introduction: symmetry; operations & elements, point groups, crystallographic and non-crystallographic point groups, assigning point groups, definition and properties of a group, subgroups, group multiplication table, matrix representation of a group, character tables. The great orthogonality theorem, rules derived from the theorem, developing of character tables for various point groups, matrices, matrix multiplication, character of a matrix, reducible representations and their reduction, symmetry and physical properties of molecules.

Application of group theory: to valence bond theory and hybrid orbitals, crystal field theory and Jahn-Teller distortion, MX_n molecules with pi-bonding, pi-bonding in aromatic ring systems, vibrational spectroscopy, molecular vibrations using internal coordinates, bonding modes, geometric isomers, infrared and Raman active vibrations, exclusion rule, molecular orbital diagrams, metal sandwich compounds and AB_n molecules.

4. Text /Reference Books

- a. A. Vincent, *Molecular Symmetry and Group Theory*, 2nd Ed., Wiley (2000).
- b. K.C. Molloy, *Theory for Chemists: Fundamental Theory and Applications*, 2nd Ed., Woodhead Publishing in Materials (2011).
- c. L.R. Carter, *Molecular Spectrometry and Group Theory*, John Wiley and Sons (2004).
- d. F.A. Cotton, *Chemical Applications of Group Theory*, 3rd Ed., Wiley India (2008).
- e. A.B.P. Lever, *Introduction to Electronic Spectroscopy*, 2nd Ed., Elsevier, Amsterdam (1984).