Course No.	Course Name	L-T-P-Credits
CY 406	**Symmetry and Group Theory**	**3-0-0: 03**
Prerequisite: NIL		

Course Objectives: The main objective of the course is to provide basic knowledge of group theory and its role in Chemistry. The course targets to explain symmetry elements and point group of molecules, to examine the group multiplication table, to explain the procedure of formation of Character Table, and to examine the application of group theory in spectroscopy, molecular vibration, ligand field theory, etc.

Course Outcomes: After successful completion of the course, students will be able to:

1. Understand the basics of Group theory
2. Identify the symmetry elements present in a molecule and the point group of the molecule
3. Formulate the group multiplication table
4. Estimate the number of subgroups, classes present in the point group of the molecule
5. Construct the character table of C_{2v}, C_{3v} and other smaller point group
6. Understand the relevance of group theory in Quantum chemistry in terms of Symmetry Adopted Linear Combination (SALC)
7. Learn the spectroscopic selection rule in terms of symmetry of a molecule
8. Find out the symmetry of translational, rotational, and vibrational modes of a molecule and also IR and/or Raman active modes
9. Learn the ligand-field theory from symmetry point of view and understand the correlation diagram of d^n systems.

SYLLABUS

Module	Contents	Hours
I	**Introduction** Symmetry operation, elements of symmetry, matrix representation of symmetry operations, definition of Group, products of symmetry operations and group multiplication table, classification of groups, point groups of molecules and their identifications.	10
II	**Orthogonality Theorem** Reducible and irreducible representations, character tables for molecular point groups, direct product representation and its applications, symmetry adapted linear combination (SALC) for C_{2v}, C_{3v}, D_{4h} and T_d, O_h point group molecules.	06
III	**Chemical Applications of Group Theory** Use of group theory in construction of hybrid orbitals: Hybridization, identification of atomic orbitals taking part in hybridisation of trigonal planar, square planar, trigonal bipyramidal, square pyramidal and tetrahedral molecules, molecular symmetry and optical activity.	08

IV	**Ligand Field Theory** Symmetry aspects of splitting of d-orbitals in different environments, electron repulsion in many electron system, term symbols, spin- orbit coupling, construction of energy level diagrams in Oh and Td symmetries, Correlation diagram, Tanabe-Sugano diagrams. Selection rules for electronic spectra. Molecular orbital theory of complex compound, LGO and MO's of octahedral and tetrahedral complexes	08
V	**Molecular Vibrations** Symmetry of vibrations, selection rules for IR and Raman spectra	04

Essential Readings:

1. F. A. Cotton, "Chemical Applications of Group Theory", John Wiley and Sons Ltd., 3rd Edition, 2008.
2. R. L. Carter, "Molecular Symmetry and Group Theory", Wiley, 1st Edition, 2009.

Supplementary Readings:

1. G. Davidson, "Introductory Group theory for Chemists", Elsevier Publishing Company Ltd.
2. A. Vincent, "Molecular Symmetry and Group Theory", John Wiley and Sons Ltd., 2nd Edition, 2000.