Course Type	Course Code	Name of Course		Т	P	Credit
DC	NCYC512	Group Theory	3	1	0	4

## **Course Objective**

- This course will impart
- The fundamental understanding of symmetry elements and operations
- Basic principles of group theory
- Applications of group theory in spectroscopy.

## **Learning Outcomes**

- After studying this course, students should be able to:
- Symmetry of the molecules and the symmetry operations therein.
- Interpret whether a given group is Cyclic, Abelian and/or given a finite Cyclic group.
- Understand the construction and use of character tables in electronic and vibrational spectroscopy.
- Understand the techniques in group theory to interpret electronic spectra in transition metal complexes.

Unit No.	Topics to be Covered	Lecture Hours	Learning Outcome
1	Symmetry elements and symmetry operations, Algebraic Operators, Point groups and its determination in various molecules. Matrix mathematics & Matrix representation symmetry operations, Eigenvalues and eigenvectors, Similarity transformation of matrices, Diagonalization of matrices.	13L + 5T	After studying this unit, the students should be able to: Symmetry of the molecules and the symmetry operations therein.
2	Definition of a Group, Subgroup, Abelian group, Cyclic group. Rearrangement Theorem, Group multiplication Tables, Lagrange's Theorem. Classes, Direct Products, Reducible & Irreducible representations. The Great Orthogonality Theorem and its consequences. Character table & its construction, Standard reduction formula, Symmetry of Translations and rotations. Symmetry of p and d orbitals.	14L + 4T	In this unit the students can interpret whether a given group is Cyclic, Abelian and/or given a finite Cyclic group. They will also learn the construction and use of character tables.
3	Classification & Determination of normal vibrational modes, Transition moment integral and selection rules. Projection operator, Application to atomic orbitals, molecular orbitals, hybridization, LCAO Approximation, π-electron	15L + 5T	The students will use character tables in electronic and vibrational spectroscopy. They will learn the techniques in group theory to interpret electronic spectra in transition metal complexes.

approximation, Hückel $\pi$ -orbital method and applications. Construction of SALCs for different geometry of molecules. SALCs for $\sigma$ and $\pi$ bonding. Molecular orbitals of sandwich compounds.		
Total	42L+14T	

## **Text Books:**

1. Chemical Applications of Group Theory, F. A. Cotton, 3<sup>rd</sup> Edition, John Wiley & Sons, 2008.

## **Reference Books:**

- 1. Symmetry and Group Theory in Chemistry, S. K. Dogra and H. S. Randhawa, 1st Edition, New Age International Publishers, 2014.
- 2. Symmetry in Bonding and Spectra (An Introduction), B. E. Douglas, C. A. Hollingsworth · Academic Press, 2012