NOC:Chemical Applications of Symmetry and Group Theory - Video course

COURSE OUTLINE

The aim of this course is to provide a systematic treatment of symmetry in chemical systems within the mathematical framework known as group theory. Once we have classified the symmetry of a molecule, group theory provides a powerful set of tools that provide us with considerable insight into many of its chemical and physical properties. Some applications of group theory that will be covered in this course include:
(i) Predicting whether a given molecule will be chiral, or polar;
(ii) examining chemical bonding and visualizing molecular orbitals;
(iii) predicting whether a molecule may absorb light of a given polarisation, and which spectroscopic transitions may be excited if it does;
(iv) investigating the vibrational motions of the molecule, etc.

COURSE DETAIL

Week	Topics
1.	Introduction; Mathematical definition of a group, Symmetry operations and symmetry elements
2.	Symmetry classification of molecules – point groups, symmetry and physical properties: Polarity, Chirality etc.;
3.	Combining symmetry operations: ‘group multiplication’ Review of Matrices, Matrix representations of groups with examples
4.	Properties of matrix representations: Similarity transforms, Characters of

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Chemistry and Biochemistry

Pre-requisites:

Basic knowledge of quantum mechanics would be helpful.

Coordinators:

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	representations, Irreducible representations (IR) and symmetry species, character tables
5.	Reduction of representations: The Great Orthogonality Theorem; Using the GOT to determine the irreducible representations spanned by a basis
6.	Symmetry adapted linear combinations, bonding in polyatomics, constructing molecular orbitals from SALCs, calculating and solving the orbital energies and expansion coefficients
7.	Molecular vibrations : determining the number of vibrational normal modes, determining the symmetries of molecular motions, Molecular vibrations using internal coordinates
8.	Spectroscopy –Group theory and molecular electronic states, electronic transitions in molecules, vibrational transitions in molecules, Raman scattering. Summary of the course

References:

1. “Chemical Applications of Group Theory” by F. A. Cotton; Third Edition, Wiley.
2. “Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications” by Alan Vincent; 2nd Edition, Wiley.
3. “Symmetry and Spectroscopy” by D. C. Harris and M. D. Bertolucci; Dover publications.