CHEMICAL APPLICATIONS OF SYMMETRY AND GROUP THEORY

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TYPE OF COURSE : Rerun | Elective | UG/PG
COURSE DURATION : 8 weeks (24 Jan' 22 - 18 Mar' 22)
EXAM DATE : March 27, 2022

PRE-REQUISITES : Basic Knowledge of quantum mechanics would be helpful.

INTENDED AUDIENCE : Senior UG and PG students

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:

1. Predicting whether a given molecule will be chiral, or polar;

2. Examining chemical bonding and visualizing molecular orbitals;

3. Predicting whether a molecule may absorb light of a given polarisation, and which spectroscopic transitions may be excited if it does;

4. Investigating the vibrational motions of the molecule, etc.

ABOUT INSTRUCTOR :

Prof. Manabendra Chandra is an assistant professor in the Department of Chemistry at IIT Kanpur. His area of specialization is experimental physical chemistry.

COURSE PLAN :

Week 1 : Introduction; Mathematical definition of a group, Symmetry operations and symmetry elements

Week 2 : Symmetry classification of molecules – point groups, symmetry and physical properties: Polarity, Chirality etc.;

Week 3 : Combining symmetry operations: ‘group multiplication’ Review of Matrices, Matrix representations of groups with examples

Week 4 : Properties of matrix representations: Similarity transforms, Characters of representations, Irreducible representations (IR) and symmetry species, character tables

Week 5 : Reduction of representations: The Great Orthogonality Theorem; Using the GOT to determine the irreducible representations spanned by a basis

Week 6 : Symmetry adapted linear combinations, bonding in polyatomics, constructing molecular orbitals from SALCs, calculating and solving the orbital energies and expansion coefficients

Week 7 : Molecular vibrations : determining the number of vibrational normal modes, determining the symmetries of molecular motions, Molecular vibrations using internal coordinates

Week 8 : Spectroscopy –Group theory and molecular electronic states, electronic transitions in molecules, vibrational transitions in molecules, Raman scattering. Summary of the course