SYMMETRY AND GROUP THEORY

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PRE-REQUISITES : General Physical Chemistry, Fundamentals of Spectroscopy

INTENDED AUDIENCE : 3rd year BS-MS students, 1st year M.Sc. students with Chemistry major, 1st year Chemistry Ph.D. students

COURSE OUTLINE :

The objective of the course is to help recognize symmetry in molecules and understand its role in Chemistry. The course will explore the role of symmetry in (A) determining molecular properties (e.g. optical activity, dipole moment), (B) classifying and assigning nomenclature to molecules, molecular states and molecular motions and (C) bringing about simplifications in the application of quantum mechanics to molecules, and (D) determining spectroscopic selection rules based on molecular symmetry. Group theory applied to the study of molecular symmetry has far reaching consequences in chemistry and the course will provide an in-depth appreciation of this.

ABOUT INSTRUCTOR :

Prof. Jeetender Chugh has obtained his M.Sc. in Organic Chemistry from the University of Delhi in 2002; and his Ph.D. in Molecular Biophysics (under the supervision of Prof. R V Hosur) from the Tata Institute of Fundamental Research, Mumbai in 2008 while working in NMR Spectroscopy. He joined IISER Pune as an Assistant Professor in the Department of Chemistry and Biology in 2013 after finishing a postdoctoral fellowship at the University of Michigan, USA (mentor: Prof. Hashim M Al-Hashimi). During his tenure at the University of Michigan, He taught a course on Physical Chemistry Experiments. After joining IISER Pune, He has been teaching several theory and lab courses. He has also been teaching Introduction to NMR spectroscopy in Structural Biology at multiple departments of Savitribai Phule Pune University since 2014. He has been teaching the proposed course (Symmetry and Group Theory) at IISER Pune since Aug 2017.In this course, he will be using whiteboard to teach, with his voice over and video insert to explain.

COURSE PLAN :

Week 1: Introduction to the course; Symmetry and Parity Operator; Symmetry Elements and Operations

Week 2: Symmetry Elements and Operations; Coordinate System; Product of symmetry operations

Week 3: Symmetry Point Groups; Schönflies Notations of the Point Groups; Point Group Determination; Applications of Symmetry - Prediction of Dipole Moment and Optical Activity

Week 4: Definition of Group, Sub-group, Class; Group Multiplication Tables; Matrix Representation of the Symmetry Operations in Point Groups

Week 5: Reducible, Equivalent, and Irreducible Representations; The Great Orthogonality Theorem and its Corollaries

Week 6: Irreducible Representations using The Great Orthogonality Theorem; Construction of Character Tables and Meaning of all the terms in the Character Table; Mulliken Symbols for Irreducible Representations

Week 7: Representations of a Cyclic Group; Application of Group Theory to Quantum Mechanics; Degenerate Eigen Functions; Direct Product of Irreducible Representations

Week 8: Applications of Direct Product, Symmetry Adapted Linear Combinations

Week 9: Projection Operator and its application to Symmetry Adapted Linear Combinations (SALCs); Symmetry and Chemical Bonding; Valence Bond Theory

Week 10: Localized and Delocalized Molecular Orbital Theory; Ascent and Descent in Symmetry

Week 11: Crystal Field Theory; Jahn Teller Distortion; Introduction to Spectroscopy; Rotational Spectroscopy

Week 12: Vibrational Spectroscopy; Raman Spectroscopy; Atomic Motions; Symmetry of Normal Modes; Visualizing Molecular Vibrations; Spectral Transition Probabilities