CHEM 583: Chemical Group Theory

INSTRUCTORS:

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Chemical Group Theory examines fundamentals and applications of group theory and representation theory to chemical problems involving molecules and crystalline solids. Students enrolled in this course will be graded on several homework problems.

Class Meeting Times: TR 1-2 PM (1222 Hach Hall); February 14-April 18, 2023

CDC COVID-19 Recommendations: CDC recommends universal indoor masking for all teachers, staff, students, and visitors, regardless of vaccination status.

Source Materials: Course materials will also be available on Canvas

Several books are placed on two-hour reserve in the Parks Library.

Chemical Applications of Group Theory, F.A. Cotton (QD 461 C65 1990)
Molecular Spectroscopy, I. N. Levine (QC 454 M6 L48)
Group Theory and Quantum Mechanics, M. Tinkham (QC 180.5 T495)

Space Groups for Solid State Scientists, G. Burns and A.M. Glazer (QC 176 B865)
Physical Chemistry of Solids, H.F. Franzen (QD 478 F73 1994)
Applied Group Theory for Chemists, Physicists and Engineers, A. Nussbaum (QD 461 N85)

Topics to be Covered:

PART 1 (Molecular): February 14-March 9 (Mark Gordon)

1. Introduction to molecular symmetry and point groups
2. Symmetry operators and commutation relations; Abelian groups
3. Construction of character tables; translations, rotations, vibrations
4. Application to electronic structure; direct products
5. Extension to non-abelian groups; classes; matrix representations
6. Reducible vs. irreducible representations; direct products revisited
7. Application to Woodward-Hoffmann rules

PART 2 (Solids): March 21-April 18 (Gordie Miller)

1. Translational symmetry: Bravais lattices and unit cells
2. Rotational symmetry with translations: Crystal systems; screw rotations; glide planes
3. Space groups: Notation; reading *International Tables*
4. Irreducible representations of the group of translations: Reciprocal space and lattices;
5. Bloch's theorem: Brillouin zones
6. Irreducible representations of space groups
7. Applications for electronic energy bands and phonons