

Chemistry 505: Group Theory in Chemistry

Textbook

Hargittai and Hargittai "Symmetry Through the Eyes of a Chemist" Plenum Press 1995.

Supplemental Reading Material:

Primary articles on course reserve in the Chemistry Library.

Cotton, Chemical Applications of Group Theory, 3rd Ed., 1990.

Burgi, H-B. and Dunitz, J. D., Structure Correlation, 1994, VCH Publ. vol 1., Ch. 1, 2 & 5.

Flurry, P. Symmetry Groups,

Wilson, Decius and Cross, Molecular Vibrations, 1955, (Dover, 1980).

Chesnut, D. B., Finte Groups and Quantum Theory, Wiley, 1974.

Course Outline:

1. Examples of symmetry groups: point groups for molecular symmetry, permutation groups for counting isomers and constructing wavefunctions, rotation groups and angular momenta
2. Classification of rigid molecules into point groups. Distinguishing isomers, geometrical and stereo-isomers.
3. Principles of Group Theory:  
matrix representations of groups; subgroup structure and faithful representations;  
character tables, projection operators, orthogonality theorem, direct products and many particle wavefunctions

Applications (selections will be based on student's interests):

4. Symmetry Control of Chemical Reactions
5. Symmetry Aspects of Molecular Orbital Theory:  
chemical bonding in planar aromatics, coordination complexes and polynuclear clusters  
state energy diagrams from electron configurations  
selection rules for electronic transitions  
configuration interaction
6. Molecular Vibrations:  
normal coordinate analysis of polyatomic molecules  
diagonalization of the classical equation of motion for harmonic vibrations  
prediction of selection rules for infrared and Raman transitions
7. Ligand Field Theory:  
the electronic configurations of the transition ions in ligand fields of varying symmetry  
consequences on magnetic properties and electronic structure

8. Structure Correlation Method

symmetry analysis of non-rigid molecules with internal degrees of freedom:  
ring deformations, axial/equatorial equilibria, Jahn-Teller distortions  
the structure correlation method for analysis of reaction paths for substitution reactions

9. Space groups: crystal symmetry