

APPLICATIONS OF SYMMETRY AND QUANTUM MECHANICS

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TEXT: **Molecular Symmetry and Group Theory**, by R. L. Carter

BOOKS ON RESERVE:

1. **Chemical Applications of Group Theory**, by F. A. Cotton, QD461.C65 1990
2. **Quantum Chemistry**, by J. P. Lowe, QP462.L69
3. **Symmetry Orbitals and Spectra**, M. Orchin and H. H. Jaffee, QD461.073
4. **Group Theory and Symmetry in Chemistry**, L. H. Hall, QD461.H17
5. **Molecular Orbital Theory for Organic Chemists**, A. Streitweiser, QD255.S88
6. **Group Theory and Quantum Mechanics**, M. Tinkham, QC174.5.T54
7. **The Conservation of Orbital Symmetry**, R. B. Woodward and R. Hoffman, QD461.W75

AIMS OF CLASS:

- Understanding of how one calculates wavefunctions for polyatomic molecules and how physical and chemical properties are extracted from the wavefunctions.
- The importance of *phase* (relative sign) in polyatomic wavefunctions.
- How group theory can be applied to the Schrödinger equation to give an exact specification of the *phase* of wavefunctions in symmetric molecules.
- How a knowledge of molecular symmetry can be applied to molecular bonding, spectroscopy, and reactivity.
- Develop a vocabulary and “experience” relevant to various aspects of your research.
- Understand “the next level” of the quantum mechanics of bonding to support your TAing and eventual professoring in undergraduate chemistry.

TOPICS TO BE COVERED:

- I. Bonding and calculations
 - A. Review of the foundations of molecular quantum mechanics
 - B. Matrices

- C. Molecular orbitals for polyatomic molecules
 - 1. Variation principle and the matrix formulation of quantum mechanics
 - 2. L.C.A.O. m.o. theory
 - a. Effective hamiltonians and basis sets
 - b. Huckel method
 - c. Hartree-Fock method
 - d. Application of m.o. theory in calculating electron densities, bond orders, and energies in polyatomic molecules
 - e. Hands-on m.o. calculations

- II. Group Theory and the Schrödinger equation
 - A. Theoretical basis for symmetry classification of wavefunctions
 - B. Group theoretical considerations
 - 1. Symmetry operations
 - 2. Identification of molecular point groups
 - 3. Mathematical properties of groups
 - 4. Classes, irreducible representations, character tables

- III. Application of group theory to molecular bonding
 - A. Symmetry classification of m.o.'s
 - B. Generation of SALCS
 - C. Direct products and state symmetries
 - D. Integral evaluation using symmetry
 - E. Application to metal-ligand bonding

- IV. Application of group theory to spectroscopy
 - A. Review of the semi-classical theory of spectroscopic transitions
 - B. Electronic spectra
 - 1. Transition probabilities and polarization using group theory
 - 2. Vibrational structure and the Franck-Condon Principle
 - C. Vibrational spectroscopy
 - 1. Vibrational hamiltonian and the oscillator approximation
 - 2. Normal modes and separation of translational and rotational modes
 - 3. Relevant operators and group theoretical selection rules for infrared and Raman spectroscopy

V. Other applications of group theory

A. Reactivity and the Woodward-Hoffman rules

1. Correlation diagrams
2. Non-crossing rule
3. Symmetry and reaction pathway
4. Applications

B. Optical activity

1. Basic concepts
2. Application to polynucleotide and polypeptide structure determination