CHEMISTRY 734b

Symmetry and Chemical Applications

COURSE OUTLINE 2008

Instructor: Professor Rob Lipson, Rm.1 ground floor of the Chemistry building. Office Phone: 86359
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Class Times: Wednesdays 2:30-4:30 pm in SSC 3010.

Text: There is no required text book. I take a lot of my notes from:
Robert L. Carter, Molecular Symmetry and Group Theory, John Wiley & Sons, Inc. 1998.
[QD461.C32 1998]

Additional Useful Texts
- F. A. Cotton, Chemical Applications of Group Theory (3rd ed.), [QD461.C65].
- D. Bishop, Group Theory and Chemistry, [QD455.3 G75B57].
- R. J. Flurry, Symmetry Groups, Theory and Chemical Applications, [QD455.3.M3F55].
- R. M. Hochstrasser, Molecular Aspects of Symmetry, [QD461.H59].

All these books are in the library.

Grading:		
	Problems sets	50%
	3-hour final exam (time and place TBA)	50%
	Total	100%

Course Description: An overview of Group Theory and its application to chemical problems including molecular orbitals, crystal field theory, molecular vibrations, and electronic spectroscopy.

Course Content (subject to change)

1. Elementary Properties of Groups: Definitions, multiplication tables, conjugate elements and classes, subgroups, mappings and homomorphism.

2. Symmetry and Point Groups: Definitions, the symmetry point groups, identification of molecular point groups.

3. Matrix Representations: Linear vector spaces, matrix representations of operators, mappings, transformation of scalar functions, some quantum mechanical considerations.

4. Group Representations: Irreducible representations, characters, the Orthogonality Theorem and its consequences, properties of characters, reduction of a representation, character tables, their structure and use, transformation of operators, basis functions, projection operators, direct product representations, operators as bases, matrix elements.

5. Molecular Orbitals: Benzene - an example of a π-electron system; use of zero-overlap and Hückel approximation; hybridization: AB_4, AB_5, symmetry orbitals; bond-orbital transformations using NO_3 as an example; transition metal complexes: The O_h complex as an example: MOs for σ- and π-bonding. Diels Alder reactions.

6. Crystal Field Theory: Russell-Saunders coupling in free ions, effects of intermediate and strong fields on d^2 configuration in O_h symmetry, as an example; lower symmetries, use of the method of descending symmetries to determine spin states, correlation tables and correlation diagrams.

7. Molecular Vibrations: Symmetries of normal modes; allowed infrared and Raman transitions, use in the elucidation of structure.

8. Electronic Transitions and Electronic Spectra: Review of non-zero matrix element condition, analysis of benzene spectra and some transition metal complexes, vibronic coupling, Jahn-Teller effect, polarization, charge transfer.

9. Spin-orbit Coupling and Double Groups: effect of spin-orbit coupling on Russell-Saunders states, the J quantum number, the character for half-integer J, double groups and their class structure, characters for double group representations, Russell-Saunder state splittings in medium and weak fields, correlation diagrams.