Chemistry 689
A Brief Introduction to Symmetry and Group Theory in Chemistry

Instructor: Dr. Timothy Hughbanks
Time: TTh 12:45 - 2:00 PM; Room 2121
Office Hours: Tuesday 2:00 - 4:00. Other times are OK too, if I have time!

Texts:
(4) Handouts on the class web site are required reading. Of these, those followed most closely are:
    (a) Survival Facts from Quantum Mechanics
        (www.chem.tamu.edu/rgroup/hughbanks/courses/673/handouts/qm_notes.pdf)
    (b) Perturbation Theory and Subgroups
        (http://www.chem.tamu.edu/rgroup/hughbanks/courses/673/handouts/subgroups&perturbation_theory.pdf)
    (c) Antisymmetric Wavefunctions: Slater Determinants
        (www.chem.tamu.edu/rgroup/hughbanks/courses/673/handouts/antisymmetry.pdf)

The course provides a shortened introduction to the fundamentals and applications of the theory of group representations in chemistry. The content of the course will be narrowed compared with our current Chem 673 to accommodate a later development of modular format of Chem 673. After a brief introduction to the abstract theory of groups is given, applications of symmetry groups will constitute the major emphasis of the course. The student will be encouraged to develop both the formal skills of using group theory to “grind out answers” and to acquire some intuitive and pictorial sense of “what it all means”. For the more mathematical (formal) first third of the course, the lectures will probably more closely follow the text than the second half. For many topics, particularly with aspects of quantum mechanics and those dealing with solids, additional handouts and reference materials are necessary and available.

Grades will be based on the homework (≈ 33%), midterm and final exams. The anticipated point breakdown should go as follows: 5 problem sets (normalized to 30 pts each), one midterm exam (100 pts), and a final exam (200 pts). Students are expected to make a serious attempt at every assigned homework problem before consulting with
peers, otherwise collaboration is permitted as long as significant contributions are made
by all collaborators. *Do not expect to be able to do all problems in a problem set in a
single sitting.*

**Module #1 – required of all students**  
**10 lectures**

I. Basic Properties of Groups and Symmetry Groups  
~ 2 weeks
A. Multiplication of elements  
closure, existence of an identity element and reciprocals, associative law  
noncommutation of operations  
multiplication tables  
subgroups and supergroups
B. Symmetry groups  
symmetry elements and operations  
assigning point groups (flow chart)  
examples of subgroups  
abelian groups, cyclic groups
C. Similarity transformations and classes  
similarity transformations  
geometrical significance of classes of symmetry operators

II. Group Representations and Physical Implications  
~ 3 weeks
A. Matrices as representations for symmetry operations  
review of vector and matrix properties; matrix operations  
some special properties of matrices  
character (trace) of a matrix  
orthogonal matrices, matrices as geometric transformation operators  
inverses
B. Group representations  
reducible and irreducible representations  
the “Great Orthogonality Theorem” and its consequences  
character tables  
cyclic groups
C. Group theory as a tool in quantum mechanics  
operators in quantum mechanics  
the importance of operators that commute with the Hamiltonian  
symmetry operators as special cases of commuting operators  
the direct product and its uses  
bases for group representations and nonzero matrix elements  
transition probabilities – including application to selection rules for vibrational  
spectra (IR and Raman single quantum transitions, i.e., fundamentals)
D. Symmetry-Adapted Linear Combinations (SALCs) and Bases for Irreducible Representations.
   projection operators and the construction of SALCs
   symmetry patterns, SALCs, and the intuitive nature of bases for irreducible representations - a pictorial survey, Mulliken notation

III. Selected Applications: MO Theory, Vibrational Spectra ~ 3 weeks

A. Molecular Orbitals in Organic Molecules (Hückel Theory – a quickie version)
   the LCAO method - secular determinants and the Hückel approximation
   MO diagrams
   using group theory to “block factor” secular determinants
   carbocyclic molecules and other examples of \( \pi \) bonding
   \( \pi \) carbon-based chains and layers (e.g., polyacetylene and graphite)
   more examples (e.g., heteroatoms, pericyclic reactions, etc.)

B. Molecular Orbitals in Inorganic Molecules
   MOs for octahedral and tetrahedral molecules
   other molecular shapes (trigonal prisms, low coordination numbers)
   Some basics of ligand field theory (some spin worries)

C. Molecular Vibrations
   normal modes
   symmetries of normal modes
   mixing of internal coordinates in normal modes
   selection rules for vibrational spectra (IR and Raman)
   mixing of internal coordinates in normal modes

D. Ligand Field Theory (Some spin worries)
   atomic states
   connecting atomic states and molecular states
   Slater determinants as bases for reducible and irreducible representations
   high-spin and low-spin molecules
   Jahn-Teller effects - applications of subgroups
   selection rules for electronic transitions in molecules
   selection rules for electronic transitions in solids
   vibronic coupling and the solid state analog, electron-phonon coupling
### Chemistry 673 - Other Suggested Books (more advanced texts in italics)

<table>
<thead>
<tr>
<th>Author(s)</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ballhausen</td>
<td>Introduction to Ligand Field Theory</td>
</tr>
<tr>
<td>Ballhausen</td>
<td>Q. M. and Chemical Bonding in Inorganic Complexes</td>
</tr>
<tr>
<td>Bishop</td>
<td>Group Theory and Chemistry</td>
</tr>
<tr>
<td>Burdett</td>
<td>Molecular Shapes</td>
</tr>
<tr>
<td>Albright, Burdett, Whangbo</td>
<td>Orbital Interactions in Chemistry, 2nd Edition</td>
</tr>
<tr>
<td>Burns &amp; Glazer</td>
<td>Space Groups for Solid State Scientists</td>
</tr>
<tr>
<td>Butler</td>
<td>Point Group Symmetry Applications</td>
</tr>
<tr>
<td>Figgis</td>
<td>Introduction to Ligand Fields</td>
</tr>
<tr>
<td>Flurry</td>
<td>Symmetry Groups</td>
</tr>
<tr>
<td>Franzen</td>
<td>Physical Chemistry of Solids, Basic Principles …</td>
</tr>
<tr>
<td>Hanna</td>
<td>Quantum Mechanics in Chemistry</td>
</tr>
<tr>
<td>Hoffmann</td>
<td>Solids and Surfaces, A Chemist's View…</td>
</tr>
<tr>
<td>Heine</td>
<td><em>Group Theory in Quantum Mechanics (Dover)</em></td>
</tr>
<tr>
<td>Kettle</td>
<td>Symmetry and Structure</td>
</tr>
<tr>
<td>Lax</td>
<td><em>Symmetry Principles in Solid State and Molecular Physics</em></td>
</tr>
<tr>
<td>McQuarrie &amp; Simon</td>
<td>Physical Chemistry</td>
</tr>
<tr>
<td>Molloy</td>
<td>Group Theory for Chemists</td>
</tr>
<tr>
<td>Murrell, Kettle &amp; Tedder</td>
<td>The Chemical Bond</td>
</tr>
<tr>
<td>Molloy</td>
<td>Group Theory for Chemists</td>
</tr>
<tr>
<td>Pearson</td>
<td>Symmetry Rules for Chemical Reactions</td>
</tr>
<tr>
<td>Tinkham</td>
<td><em>Group Theory and Quantum Mechanics (Dover)</em></td>
</tr>
<tr>
<td>Walton</td>
<td>Beginning Group Theory for Chemistry</td>
</tr>
</tbody>
</table>

See also: