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**Course Materials:**
2) D. Snotes – about $10.
3) Molecular model kits – about $22.

**Reference Materials:**

**Goals:**
Assign molecules to their symmetry (point) groups, decide whether they are polar, chiral. Be able to interpret essentials of x-ray crystallographic results. Know the concept of a group, be able to manipulate/combine elements, use multiplication tables. Be able to use matrix representations of vectors & symmetry operations, generate simpler cases. Understand classes and subgroups, origins of character values and representations. Be able to use character tables to deduce and combine representations for various properties and objects (e.g., atomic orbitals). Know how to choose basis sets, generate & decompose representations from them & how to use projection operators. Use the Crystal Field Theory model to interrelate stereochemistry, symmetry, configuration, spin state, optical and magnetic properties and crystal field stabilization energy for transition metal compounds. [Designate terms and states, compute moments for nd and 4f ions.] Using symmetry methods, be able to derive normalized MO forms for diatomic, cyclic and centric molecules; deduce occupancy of and properties from transition metal complex MO diagrams. Generate total motional representations for molecules, deduce their infrared and Raman vibrational spectroscopic activities and correlate spectral patterns with geometry.

**Pre-Requisite Knowledge:**
Inorganic-I: s,p,d,f-Atomic orbitals; configurations of nd cations; VSEPR; qualitative MO concepts; symmetry elements. PChem: infrared and electronic (optical) absorption phenomena.

**Other stuff:** Be sure that I have your correct Email address for my exploder. Work on the problem sets !! Attempt to solve the homework problems as soon as we have covered the material in class. There is no grade given for attendance or for homework. If you do not do the homework, you will find it hard to pass the exams, and virtually impossible to get a good
grade. I suggest that you form a study group with some like-minded students in the course, and collaborate in studying and problem-solving. For help with problem sets, I may be found in my office or lab most of the daytime during the week. Your grade is based on the (usually three) exams: two midterms (15%, 25%) plus a final exam (60%). You may bring our periodic table and molecular model kit to the exams. Some of the assigned classrooms have no periodic table.

Make-Up Exams?
You don't need an excuse to take the make-up exam if you miss a midterm or final, but you must then attend the make-up at the designated time and place or take a zero on it - no excuses. Make-up exams are of equal or greater difficulty than the ones they replace. All make-up exams are intended to be on Monday March 20th at 3:00 pm in 12-307.

The 10-Minute Rule: If I'm more than ten minutes late without prior notice, consider the class cancelled. If you are going to be more than ten minutes late for a class, please don't enter without prior arrangement, until the class takes a break.

0. [Nomenclature]*
1. Point groups and the assignment of molecules to them.
2. Immediate applications: [dipole moments,] asymmetry, dissymmetry, chirality.
3. Elements of crystal symmetry; interpretation of diffraction articles.
4. Elements and groups: general properties, combination, multiplication tables.
6. [Similarity transforms, conjugation, classes,*] Matrix representation of 3D vector.

Crystal Field Theory.
12. Jørgensen’s f & g; spin states & magnetism of nd systems [4f systems, spin crossover, binuclear complexes,*].
13. CFSE & stability, $T_d$ fields, 4d- & 5d-ions; planar/D$_{4h}$ symmetry.
15. MO’s for $H_2$: from basis set to representation. Other diatomics’ MO’s.
16. Decomposition formula; MO’s for cyclic tetraatomic ($S_4^{4+}$ p-system): SALC’s.
17. Projection operators. Use of PRSG, normalisation & relative energies of MO’s.
18. Symmetry factoring for centric molecule: LGO’s, s & p MO’s for BF$_3$.
21. $\Gamma_T \rightarrow \Gamma_{T,R,\text{Rot,}Vib}$-infrared & Raman activity selection rules.
22. Effects of coordination: correlation tables.
24. Raw AO’s as normalised functions of hybrids, matrix representation, transposition & inversion.

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