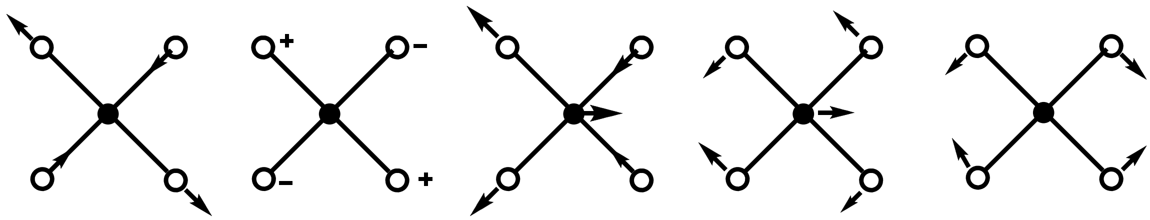
5.04 Principles of Inorganic Chemistry II
Fall 2008

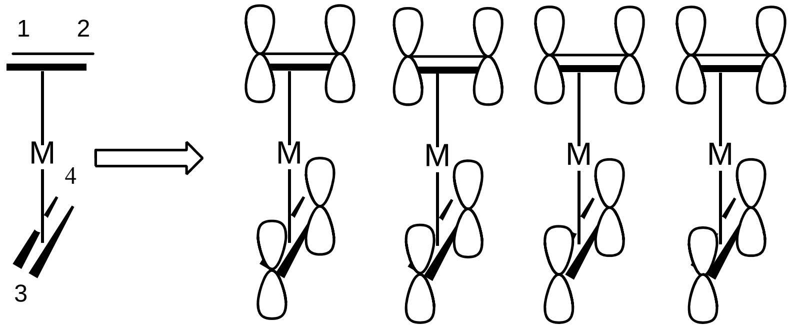
100 points total

1. (**20 pts**) Below are vibrations and orbitals of molecules that transform according to irreducible representations of their given point groups. Note: no derivations are needed to answer this problem.

   a. (**10 pts**) Five bending modes of XeF_4^{2-} are shown below. Assign the modes to their appropriate irreducible representations.



   b. (**10 pts**) Olefins can bind to metal centers. Consider the simplets homoleptic complex, the bis(ethylene) complex. Ethylene binds to a metal through its pπ-orbitals. The four orbital symmetries appropriate for ligand binding to the metal are: A_1, B_2 and E. Below are shown the p-orbital contours for four orbitals. Color the p-orbitals to give the proper orbital symmetries. Label each of the completed diagrams with its irreducible representation



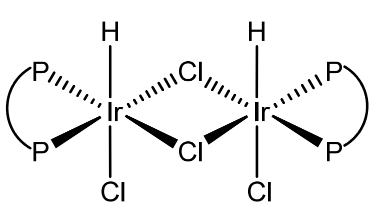
2. (**20 pts**) Show that the point groups C_{3h} and S_3 are equivalent. You may use a stereographic projection to answer this problem.

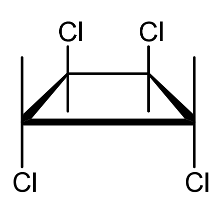
3. (**20 pts**) Short answers. Point values are assigned in parenthesis on each line.

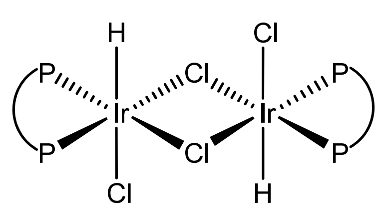
   a. (**9 pts**) Identify the point group and list the generators for the letter S

   b. (**5 pts**) To which irreducible representation does the f_{xz^2} orbital belong in the D_{2h} point group?

   c. (**6 pts**) A molecule cannot be optically active if it has any S_n axes. Identify the optically active molecules below.







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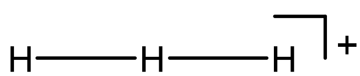
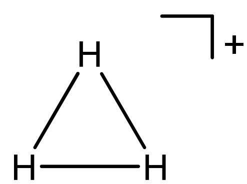
4. (**40 pts**) H_3^+ was discovered only 12 years ago by Professor Takeshi Oka of the University of Chicago. The discovery has been profound as this molecule has been observed now at the galactic core. As professor Oka discussed yesterday at MIT, the presence of this molecule in the universe provides an important mechanism for star formation. Construct an energy level diagram for the two molecules using the Hückel approximation to determine the energies. Draw a correlation diagram that relates the Hückel energy levels of the two fragments.

   To shorten the time of this problem, consider using the D_{2h} point group for the linear isomer of H_3. Also, we provide one SALC for linear H_3^+ and two SALCs for cyclic H_3^+. You need only show work for the missing SALCs.



1/√2 [H2 – H3]



1/√2 [H2 – H3]
1/√6 [2H1 – H2 – H3]