

CHEM-457 (S14)
Problem Set 2

1. Write a matrix representation for each of the following symmetry elements. (Remember, all rotations are *counterclockwise* about the z axis): (a) E (b) C_3 (c) C_4 (d) i (e) S_4

2. Assign point groups for the following. For cases in which the structure is not drawn, assume the lowest energy conformation:

(a) HF

(b) NH_3

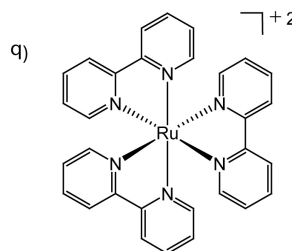
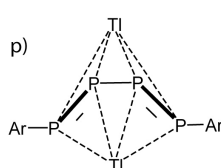
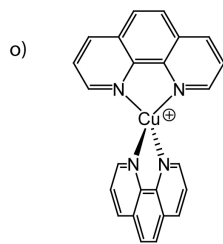
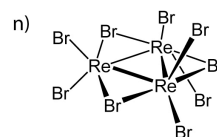
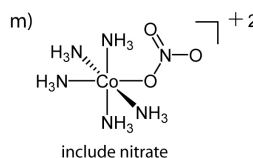
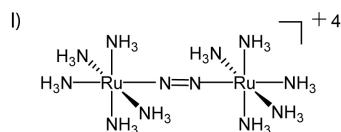
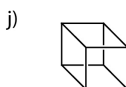
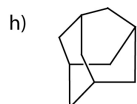
(c) Toluene

(d) $O=C=C=C=O$

(e) H_2CCCH_2

(f) $W(CO)_6$

(g) Benzene



3. Using VSEPR theory, draw Lewis structures for the following compounds, using resonance where appropriate if more than one reasonable structure is possible. Place formal charges on each atom and name the geometry of the structure.

(a) N_3^-

(b) XeF_2

(c) ClF_3

(d) PF_5

(e) I_3^-

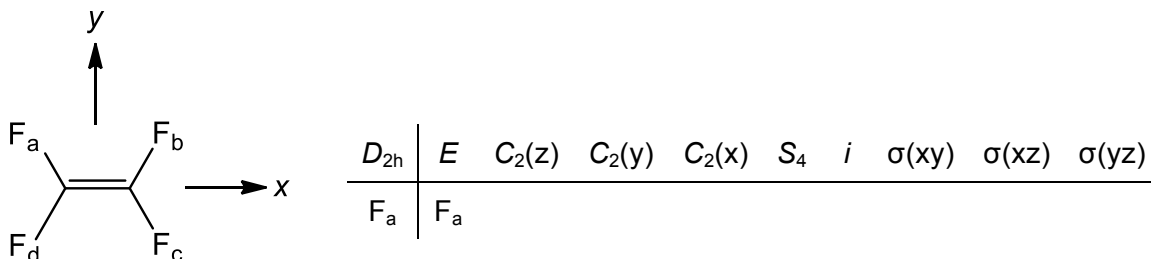
(f) CO

(g) SeF_4

(h) NO

(i) N_2O

4. Tetrafluoroethylene has D_{2h} symmetry. Using the atom labeling scheme illustrated, fill in the table to show how atom F_a transforms under each operation of the point group. Follow the sign convention introduced in lecture, where positive rotation is performed in the *counterclockwise* direction.



5. Consider the octahedral species MCl_6 , where M is a central metal. This species belongs to the point group O_h . What point group results if the symmetry is lowered upon:
- Removal of one chloride ligand
 - Replacement of one chloride ligand with a fluoride ligand
 - Removal of two *trans*-chloride ligands
 - Removal of two *cis*-chloride ligands
 - Removal of three facial chlorides
 - Removal of three meridinal chlorides
6. Draw a simple molecule that has D_{3h} point symmetry. Label the symmetry elements for this species and then construct a multiplication table for the point group.
7. Miessler, Fischer and Tarr #4.28, 4.29, 4.33 and #4.34