CHEM-651 (F14)
Problem Set 2

1. Identify and label all of the symmetry elements for the following species. Indicate whether the molecule is chiral or achiral based on the symmetry elements identified.

   (a) *trans*-1,2-difluoroethene

   (b) *cis*-1,2-difluoroethene

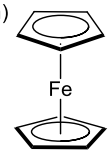
   (c) iodobenzene

   (d) *trans*-1,2-dibromocyclopropane

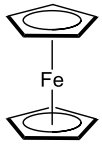
2. Assign point groups for the following. For cases in which the structure is not drawn, assume the lowest energy conformation.

(a) HF	(b) NH_3	(c) Toluene	(d) O=C=C=C=O
(e) cubane	(f) $W(CO)_6$	(g) Benzene	(h) adamantane
(i) P_4	(j) Naphthalene	(k) p-bond	(l) p-antibond

(m)

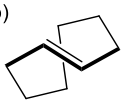


(n)



(o)

(p)



3. Cl_2 has a Cl–Cl bond length of 1.988 Å while that for Cl_2^+ is 1.8917 Å. Use Molecular Orbital Theory to rationalize these metrics and determine the bond order for each of these molecules.

4. Prepare a molecular orbital energy diagram for the cyanide ion (CN^-). Please be sure to label all atomic orbitals and molecular orbitals. Provide sketches to show how atomic orbitals interact to form MOs.

   a. Based on the MO diagram you prepared, what is the bond order of CN^-? What is the multiplicity of CN^-?

   b. Which molecular orbital of cyanide would you predict to interact most strongly with a proton in the acid-base reaction $CN^- + H^+ \rightarrow HCN$? Please explain your answer.

5. Write a Lewis electron-dot structure for N_3. Predict its molecular shape using the VSEPR method. Discuss the electronic structure N_3 in terms of hybridization at the central nitrogen atrom and the number of σ and π electrons. How many unpaired electrons are there? Is the molecule polar? Predict the relative bond lengths in N_2 and N_3.

6. We have discussed each of the following physical methods in class. Briefly describe the type of bonding/structural information each method affords.

    (a) X-Ray Diffraction

    (b) XANES

    (c) Microwave Spectroscopy

    (d) IR Spectroscopy