Chemistry 4000
Introduction to Inorganic Chemistry: The Different Perspectives of Bonding

Problem Set #2 Part B

Chapter 5-

1) a. In polyatomic molecules that contain a central atom, the number of bonds in the molecule will dictate the number of stretching vibrations that the molecule will have. Determine the symmetries for the stretching vibrations of H_2O.

b. In class I mentioned that there is a more accurate approach to determine the ligand group orbitals (LGOs) of a molecule. This approach, called the projection operator, is discussed on pages 156 of the textbook. Follow the work described on these pages to derive the LGOs for the H atoms of H_2O. YES, I literally mean write down what is written in the textbook to teach yourself this method.

c. Read problem 5.12 and refer to Table 5.6 to answer how MO theory accounts for the presence of lone pairs in H_2O.

d. Use the projection operator method to derive the LGOs of the hydrogen atoms of NH_3. Refer to pages 157-159 of the textbook for guidance.

e. Derive the MO diagram for NH_3 showing the structures of the molecular orbitals generated and the relative energies of the MO's.

2) Using the conceptual approach that we used to derive the molecular orbital diagram for BeH_2, derive the complete molecular orbital diagram for CO_2. This molecular orbital diagram must account for sigma and pi interactions. Assume that the LGOs for the 2s orbitals of the oxygens are nonbonding due to an energy mismatch.

3) Using group theory to determine the symmetries for the sigma and pi interactions of **NO_2^-**:

a. Identify which of the atomic orbitals from the central atom have symmetries that correspond with sigma interactions.

b. Identify which of the atomic orbitals from the central atom have symmetries that correspond with pi interactions.

c. Identify which of the LGOs have symmetries that correspond with sigma interactions applying a conceptual approach.

d. Identify which of the LGOs have symmetries that correspond with pi interactions using applying a conceptual approach.

e. Which orbitals will interact to form molecular orbitals? Explain in words and in drawings.

f. Are there any nonbonding orbitals?

4) Draw the molecular orbital diagram for NO_2^-.