Problem Set 6

1. Draw a molecular orbital diagram and determine the bond order expected for the molecule B_2. For full credit on MO diagrams,

- label increasing energy with an arrow next to the diagram.
- for any bonding orbital drawn, include the corresponding anti-bonding orbital, even if it is not filled with any electrons.
- Label each atomic orbital and each molecular orbital that you draw.
- Fill in the electrons for both the atomic and molecular orbitals

2. The dissociation energy of N_2 is 942 kJ/mol, whereas that for N_2^+ is 842 kJ/mol. The dissociation energy of O_2 is 494 kJ/mol, whereas that for O_2^+ is 642 kJ/mol. Rationalize these data.

3. Sketch an MO diagram for BeH. On the basis of your diagram, would you expect this molecule to be stable with respect to dissociation into atoms.? Use your MO diagram to predict any other properties you can.

4. Draw the π and π^* MO's for N_2 and CO. Qualitatively show the difference. Comment on the contribution from individual AO's in the resulting MO's.

5. Consider that the orbital structure of the heteronuclear diatomic ion NO^+ is similar to that of N_2. Use this information to draw the energy level diagram for NO^+. In the molecular orbital, will the electrons have a higher probability of being at N or at O? Why?

6. Photoelectron spectrum of a second row homonuclear diatomic molecule was recorded using 21.21eV photons. It is observed that K.E_{max} of the ejected electrons from the top three HOMO's were 10.01, 8.23, and 5.22 eV, having intensity ratios of 1:2:1. Sketch the molecular orbital energy level diagram and identify the possible molecule(s).