Name ___________________________ Test 3 (11/16)
CHEM 0211 (Adv. Inorganic) Fall 2012

1. (12 pts.) In order to form an MO from AO's three things need to be true about the AO's. Those three things are...

1. ________

2. ________

3. ________

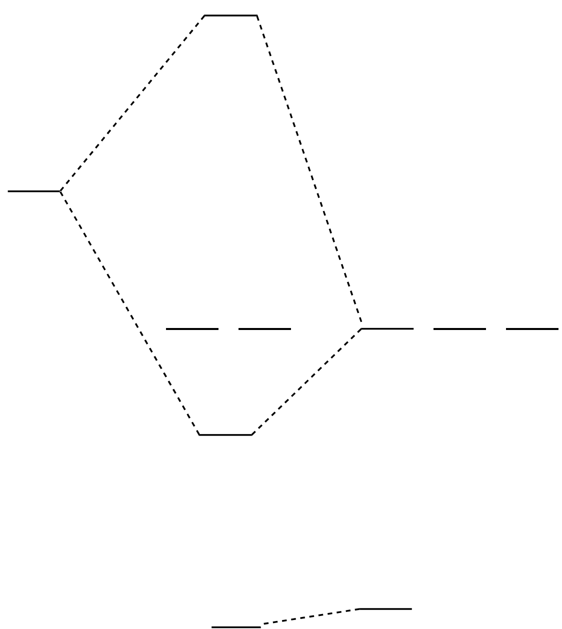
4. ________

2. (10 pts.) In general, p_x orbitals interact with other p_x orbitals, they do not tend to interact with p_y or p_z orbitals. Explain.

5. ________

6. ________

3. (24 pts.) A partial MO diagram for HF is drawn below.



a. Complete the diagram by labeling the atomic orbitals and adding the appropriate number of e⁻'s to the atomic and molecular orbitals.

b. Label the LUMO.

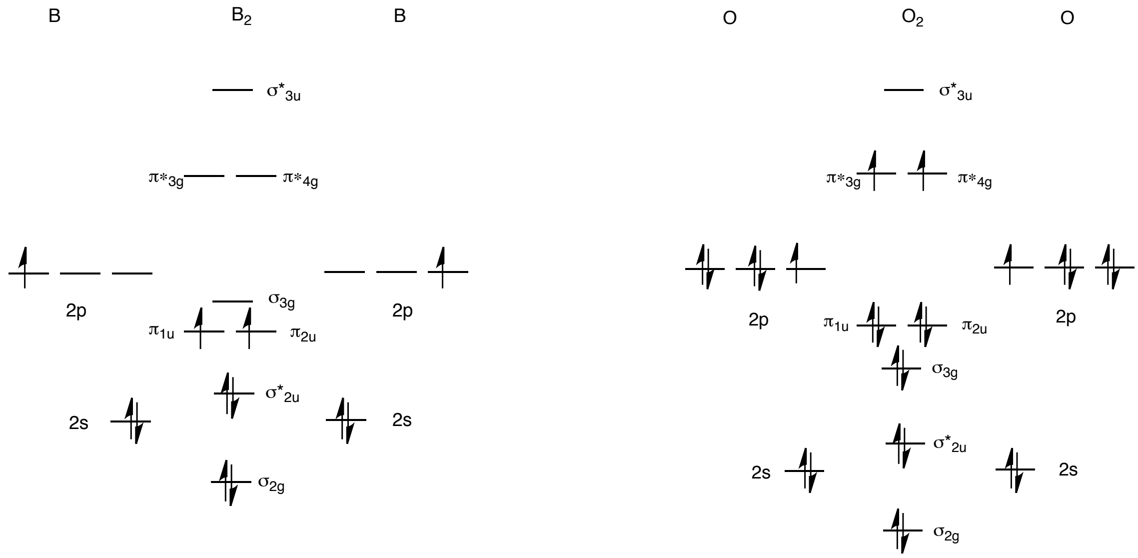
c. Label the HOMO.

d. i. If an electron donor reacts with HF, to which orbital would the e⁻'s be added?

d. ii. The orbital that is receiving the e⁻'s in d.i. would more strongly resemble which atom, the F or the H?

e. Label bonding, non-bonding, and antibonding orbitals.

4. (16 pts.) MO diagrams for B_2 and O_2 are drawn below. Note that even though the energies of the orbitals are not drawn to scale, the position of the σ_{3g} orbital is correctly drawn below the π orbitals on O_2 and the σ_{3g} orbital is drawn above the π orbitals on B_2. The changing position is a result of differing amounts of mixing on B_2 as compared to O_2.



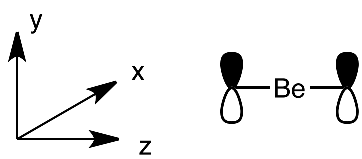
a. The term "mixing" refers to the mixing of what orbitals?

b. Why is the order of the orbitals different on the two molecules, in other words, why is the mixing strong in one molecule as compared to the other?

5. (16 pts.) The point group for BeF_2 is $D_{\infty h}$, but when determining the symmetry of the group orbitals formed from the F atoms it is more convenient to use the D_{2h} point group.

D_{2h}	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	i	$\sigma_h(xy)$	$\sigma_d(xz)$	$\sigma_d(yz)$		
A_g	1	1	1	1	1	1	1	1		x^2, y^2, z^2
B_{1g}	1	1	-1	-1	1	1	-1	-1	R_z	xy
B_{2g}	1	-1	1	-1	1	-1	1	-1	R_y	xz
B_{3g}	1	-1	-1	1	1	-1	-1	1	R_x	yz
A_u	1	1	1	1	-1	-1	-1	-1		
B_{1u}	1	1	-1	-1	-1	-1	1	1	z	
B_{2u}	1	-1	1	-1	-1	1	-1	1	y	
B_{3u}	1	-1	-1	1	-1	1	1	-1	x	

A cartoon representation of the p_y orbitals on the F atoms is drawn below.

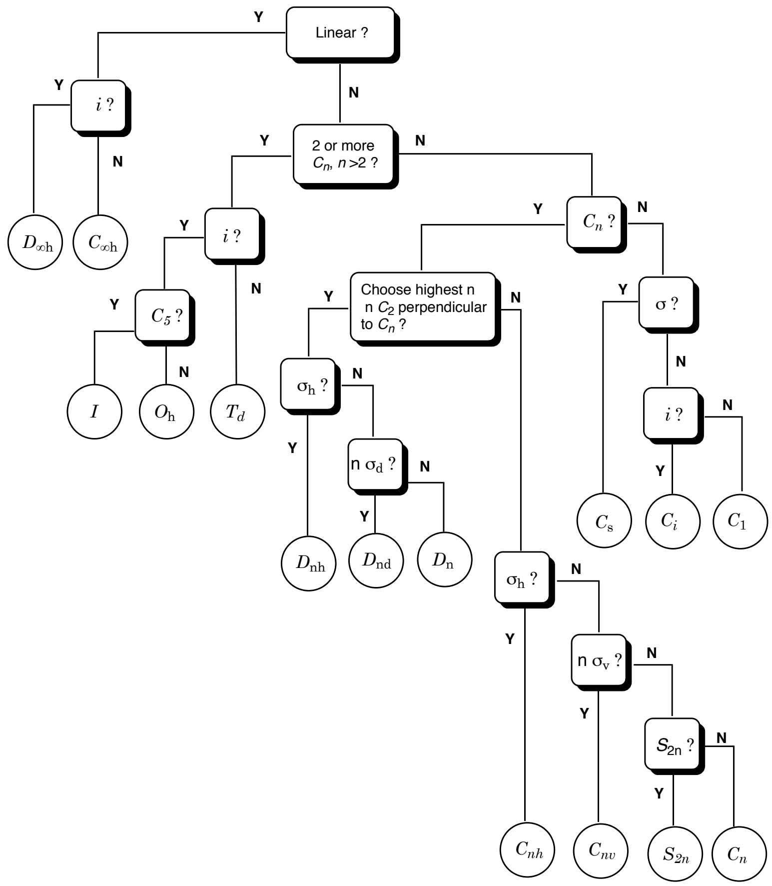


a. Determine the reducible representation for the group orbitals formed from the F atoms' p_y orbitals.

b. Determine the irreducible representations for the group orbitals formed from the F atoms' p_y orbitals.

6. (20 pts.) Create an MO diagram for BH_3. The energies for the B atom's 2s and 2p orbitals are -14.05 and -8.3 eV. The energy for the H atoms' 1s orbital is -13.61 eV.

Point Group Assignment Tree



$$\left(\begin{array}{c}\text{number of irreducible}\\ \text{representations of a given}\\ \text{type needed}\end{array}\right) = \frac{1}{\text{order}}\Sigma_{\text{classes}}\left(\begin{array}{c}\text{\# operations}\\ \text{in class}\end{array}\right)\left(\begin{array}{c}\chi\text{ of the irreducible}\\ \text{representation}\end{array}\right)\left(\begin{array}{c}\chi\text{ of the reducible}\\ \text{representation}\end{array}\right)$$

C_{3v}	E	2 C_3	3 σ_v		
A_1	1	1	1	z	$x^2 + y^2$, z^2
A_2	1	1	-1	R_z	
E	2	-1	0	(x, y), (R_x, R_y)	($x^2 - y^2$, xy), (xz, yz)

D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$		
A_1'	1	1	1	1	1	1		$x^2 + y^2$, z^2
A_2'	1	1	-1	1	1	-1	R_z	
E'	2	-1	0	2	-1	0	(x,y)	(x^2 - y^2, xy)
A_1''	1	1	1	-1	-1	-1		
A_2''	1	1	-1	-1	-1	1	z	
E''	2	-1	0	-2	1	0	(R_x, R_y)	(xz, yx)