Name _____ Test 3 (4/11)
CHEM 0211 (Adv. Inorganic) Spring 2014

1. (15 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. _____

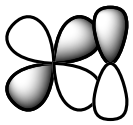
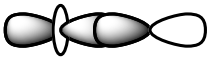
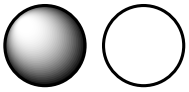
3. _____

4. _____

2. (a. 8 pts.) Determine whether the following molecular orbitals are bonding or antibonding. (c. 8 pts.) Determine the symmetry of the molecular orbitals (σ, π, δ)

5. _____

6. _____

 $3d_{xz}+2p_x$	 $3d_{xz}+2p_z$
 $2p_z - 2p_z$	 $1s - 1s$

3. (10 pts.) A 2s orbital does not have the correct symmetry to interact with a d_{xz} orbital. Explain why constructive and destructive interference is not possible between these two orbitals. You may use drawing to help make your point.

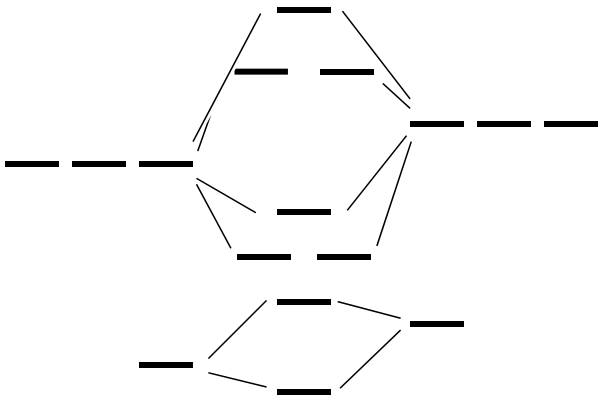
4. An incomplete MO diagram for NO^+ is provided.

a. (6 pts.) Complete the diagram by labeling the AO's (e.g., 1s, 2s, etc), labeling the MO's (e.g., σ, π*, etc) and adding the appropriate number of e^-'s to the orbitals.

b. (4 pts.) Label the LUMO.

c. (4 pts.) Label the HOMO.

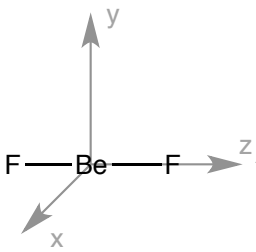
d. i. (6 pts.) If an electron donor reacts with NO^+, to which orbital would the e^-'s be added?



d. ii. (6 pts.) The orbital that is receiving the e^-'s in d.i. would more strongly resemble which atom, the N or the O? Explain.

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. (6 pts) Determine the reducible representation for the group orbitals formed from the F atoms' $2p_z$ orbitals.

b. (6pts.) Determine the irreducible representation for the group orbitals formed from the F atoms' $2p_z$ orbitals.

c. (6 pts.) Which orbital(s) on Be can interact with with the group orbitals from from the F atoms $2p_z$ orbitals, explain.

6. (12 pts.) Create an MO diagram for CH_4. The character table for the T_d point group is included below. The energy for the H atoms' 1s orbitals is –13.61 eV. The energies for the C 2s and 2p orbitals are –19.43 eV and –10.66 eV.

T_d	E	8 C_3	3 C_2	6 S_4	6 σ_d		
A_1	1	1	1	1	1		$x^2 + y^2 + z^2$
A_2	1	1	1	-1	-1		
E	2	-1	2	0	0		$2z^2 - x^2 - y^2$, $x^2 - y^2$
T_1	3	0	-1	1	-1	(R_x, R_y, R_z)	
T_2	3	0	-1	-1	1	(x, y, z)	(xy, xz, yz)

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