Name _____ Test 3 (11/25)
CHEM 0211 (Adv. Inorganic) Fall 2015

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. _____

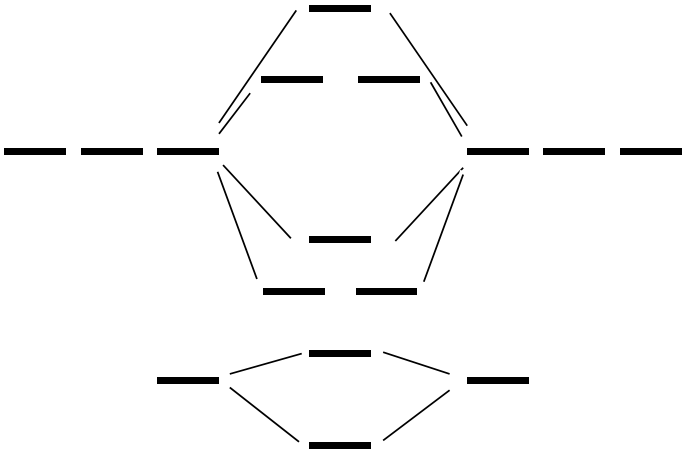
4. _____

5. _____

2. (10 pts.) In a diatomic molecule, a 2s orbital does not have the correct symmetry to interact with a $2p_y$ orbital to form a molecular orbital. Draw the interaction between a 2s and $2p_y$ orbital and explain why this pair of orbitals cannot be used to make a molecular orbital.

6. _____

3. An incomplete MO diagram for C_2 is provided.



a. (6 pts.) Complete the diagram by labeling the AO's, labeling the MO's, and adding the appropriate number of e^-'s to the orbitals.

b. (4 pts.) Label the LUMO.

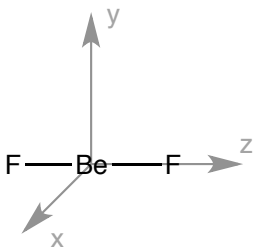
c. (4 pts.) Label the HOMO.

d. i. (6 pts.) If an electron donor reacts with C_2, to which orbital would the e^-'s be added?

d. ii. (6 pts.) Would you expect the bond between the carbon atoms to weaken if the C_2 molecule accepted a pair of electrons? Explain.

4. (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	

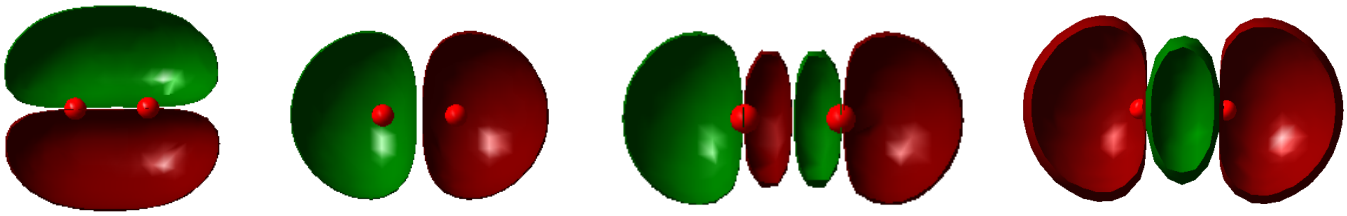


a. (6 pts) Determine the reducible representation for the group orbitals formed from the F atoms' $2p_x$ orbitals.

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

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

5. Label the following molecular orbitals from an O_2 molecule as (a. 8 pts.) bonding or antibonding, and (b. 8 pts.) g (gerade) or u (ungerade), and (c. 8 pts.) determine the symmetry of the molecular orbitals (σ, π, or δ) (the red dots represent the nuclei of the O atoms).



6. (12 pts.) Create an MO diagram for BH_3. The energy for the H atoms' 1s orbitals is –13.61 eV. The energies for the B 2s and 2p orbitals are –14.05 eV and –8.30 eV.

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)

C_{3h}	E	2 C_3	σ_h	2 S_3		
A'	1	1	1	1	R_z	$x^2 + y^2, z^2$
A''	1	1	-1	-1	z	
E'	2	-1	2	-1	(x,y)	($x^2 - y^2$, xy)
E''	2	-1	-2	1	(R_x, R_y)	(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)

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