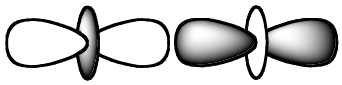
Name _____ Test 2 (10/29)
CHEM 0211 (Adv Inorganic) Fall 2010

1. When orbitals on two atoms interact constructively and destructively they form molecular orbitals.

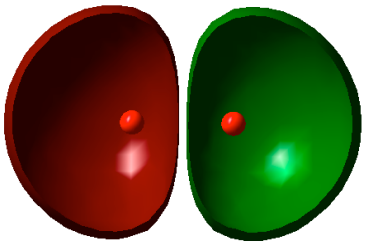
a. (8 pts.) Label the following orbitals as σ, σ*, π, or π*.

b. (10 pts.) Briefly explain (which is higher/lower and why) the relative energies of the orbitals. (Compare orbitals in a given row.)

i.



ii.



1. _____
2. _____
3. _____
4. _____
5. _____
6. _____
7. _____
8. _____
9. _____
10. _____

2. (8 pts.) In a diatomic molecule, the p orbitals can interact to form two different types of molecular orbitals. One set of molecular orbitals has σ symmetry. The other set has π symmetry. Draw examples of the σ and σ* orbitals. Draw only one orbital for each type.

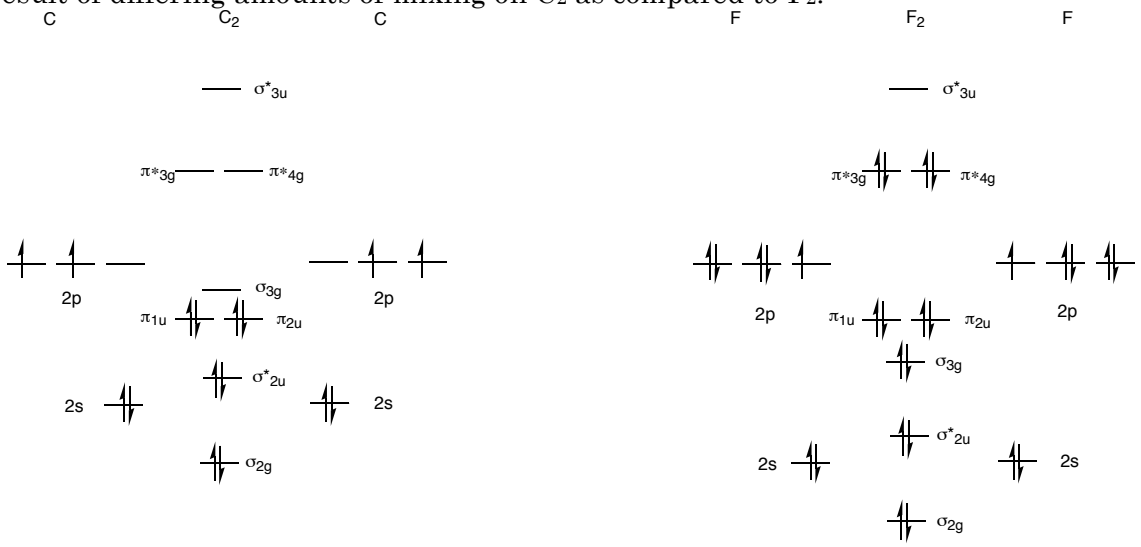
i. σ ii. σ*

3. (8 pts.) In a diatomic molecule, the p orbitals can interact to form two different types of molecular orbitals. One set of molecular orbitals has σ symmetry. The other set has π symmetry. Draw examples of the π and π* orbitals. Draw only one orbital for each type.

iii. π

iv. π*

4. (10 pts.) MO diagrams for C_2 and F_2 are drawn below. Note that the position of the σ_{3g} orbital is below the π orbitals on F_2 but the σ_{3g} orbital is above the π orbitals on C_2. The changing position is a result of differing amounts of mixing on C_2 as compared to F_2.



a. The term "mixing" refers to the mixing of what orbitals? (Describe briefly)

b. Why is the order of the orbitals different on the two molecules?

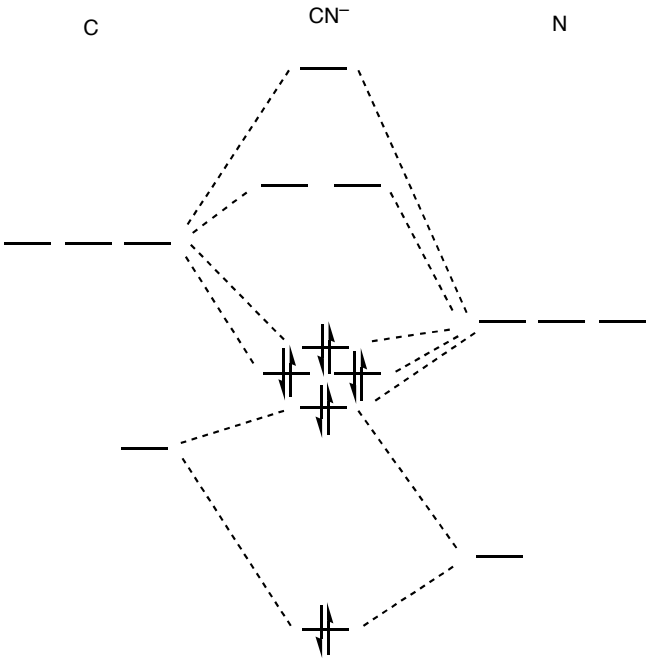
5. An MO diagram for CN^- is drawn below.

a. (3 pts.) Write "LUMO" next to the appropriate molecular orbital.

b. (3 pts.) Write "HOMO" next to the appropriate molecular orbital.

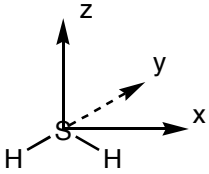
c. (4 pts.) If CN^- were to accept electrons, at which end of the molecule (the C or the N) would the new bond form?

d. Describe what factors you would consider when deciding whether the HOMO was primarily N or C based.



6. (10 pts.) When deciding whether atomic orbitals will interact to form bonding and antibonding molecular orbitals, what two properties of the atomic orbitals must be considered?

7. A Kekulé structure of H_2S is drawn below. The molecule belongs to the C_{2v} point group.



a. (6 pts.) Determine the reducible representations for the group orbitals formed from the H atoms' atomic orbitals. (The C_{2v} character table is on the next page.)

b. (6 pts.) Determine the irreducible representations for the group orbitals formed from the H atoms' atomic orbitals.

c. (6 pts.) Determine the irreducible representations for the S atom's 3s and 3p atomic orbitals.

d. Draw an MO diagram for H_2S on the following page.

C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v(yz)$		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	-1	-1	R_z	xy
B_1	1	-1	1	-1	x, R_y	xz
B_2	1	-1	-1	1	y, R_x	yz