

1. (12 pts.) Describe what each of the following symmetry operations are.

a. a σ_v operation

1. _____

2. _____

3. _____

b. a C_2 operation

4. _____

c. an E operation

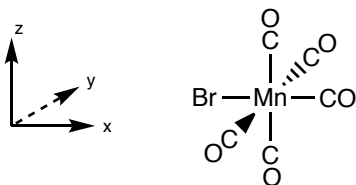
5. _____

6. _____

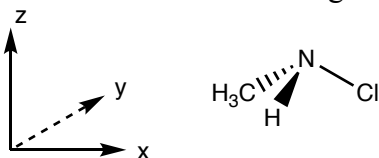
7. _____

2. (12 pts.) Perform the indicated operations on the following molecules, and draw a 3D representation, using wedge and dash notation where appropriate, for the resulting view.

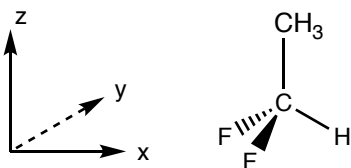
a. Perform a C_4 around the z axis that contains the Mn atom.



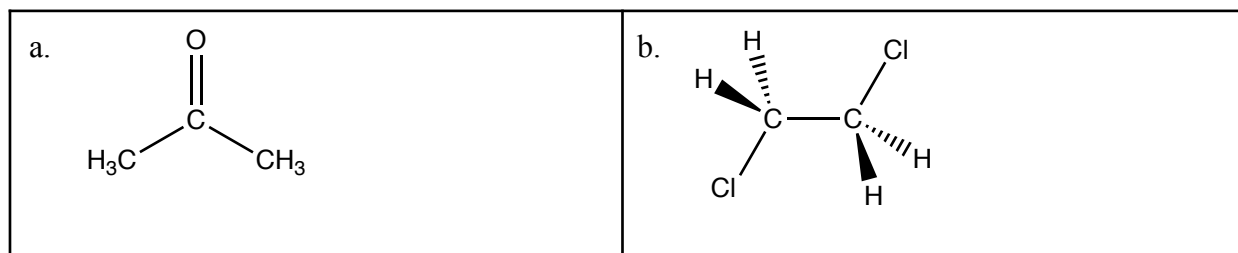
b. Perform a reflection through the xz plane that contains the N and Cl atoms



c. Perform a S_3 on the axis that contains the C to CH_3 bond.



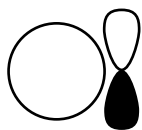
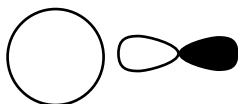
3. (16 pts.) Determine the point group for each of the following structures. Wedge and dashed 3D representations have been provided.



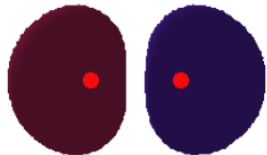
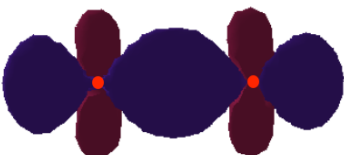
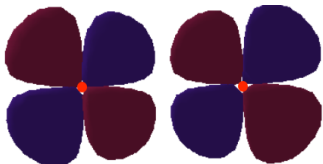
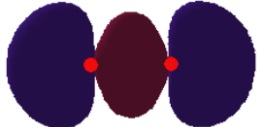
4. (10 pts.) Determine the irreducible representation for the reducible representation listed at the bottom of the following character table.

C_{3v}	E	$2 C_3$	$3 \sigma_v$		
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)	$(x^2 - y^2, xy), (xz, yz)$
Γ	3	3	1		

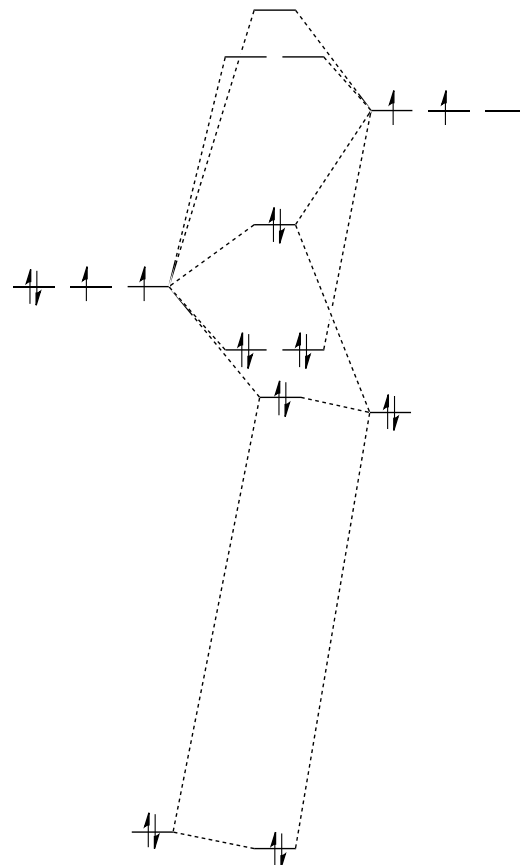
5. (10 pts.) Graphical representations of s and p orbitals appear below. Which pair will interact and form molecular orbitals. Explain your choice.



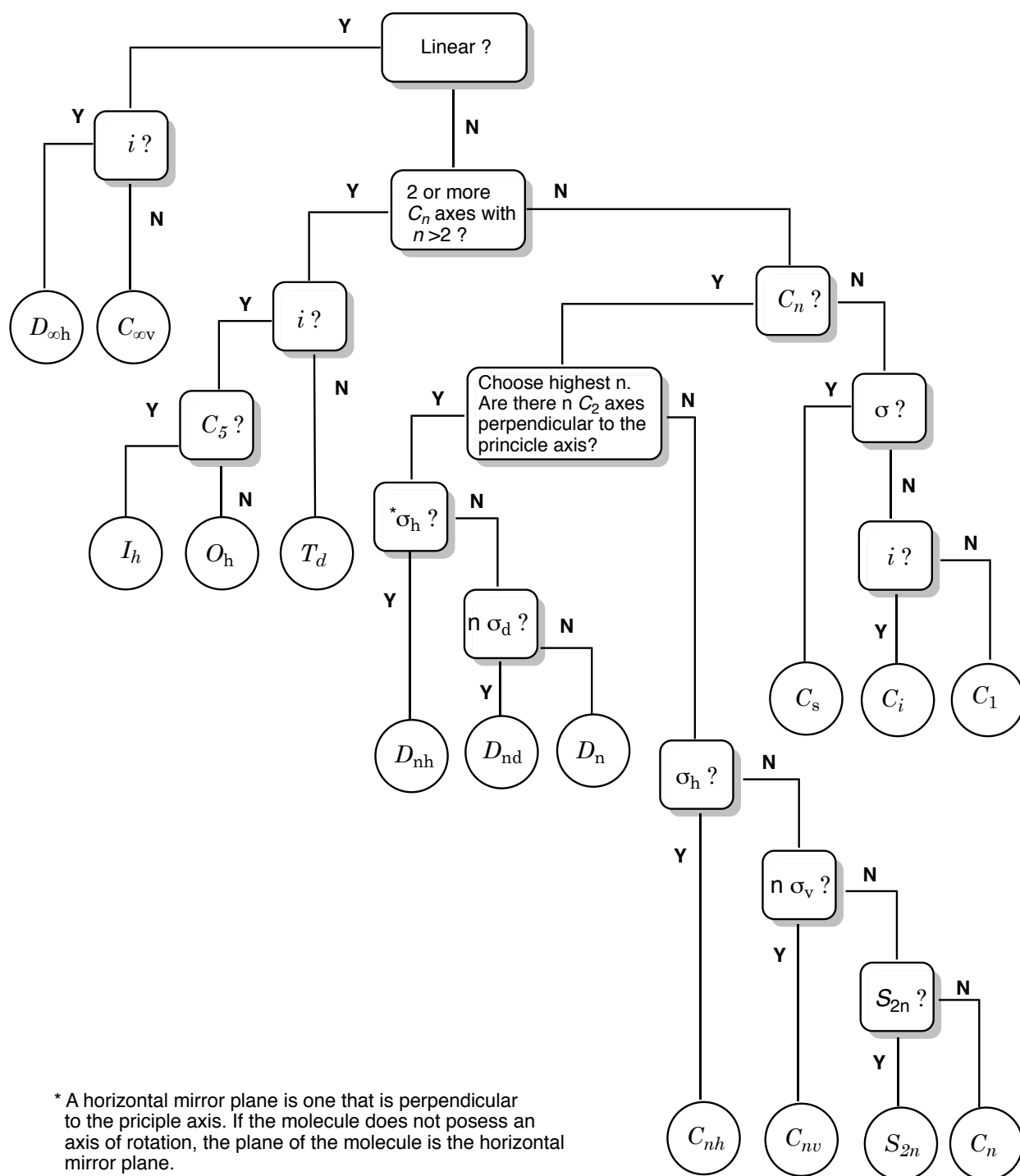
6. Graphical representations of molecular orbitals from diatomic molecules are pictured below.
- (1 pt. each) Determine whether the following orbitals would be bonding or antibonding.
 - (1 pt. each) Determine the symmetry of the orbital, σ , π , or δ
 - (1 pt. each) Determine whether the orbitals are gerade or ungerade

i. MO made from two s orbitals 	ii. MO made from two d_{z^2} orbitals 
iii. MO made from two p_z orbitals 	iv. MO made from two d_{xz} orbitals 
v. MO made from two p_z orbitals 	vi. MO made from two p_x orbitals 

7. An MO diagram for CO is drawn to the right.
- (3 pts.) Label the O and C atoms.
 - (4 pts.) Label the σ and π orbitals.
 - (2 pts.) Label the HOMO and LUMO.
 - (3 pts.) Based on the MO diagram, which end of the CO molecule is more electrophilic (willing to accept electrons), the C or O?



Point Group Assignment Tree



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