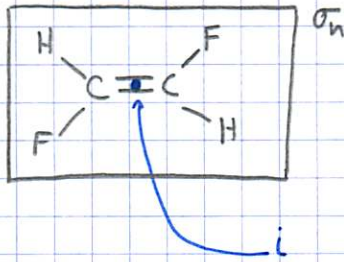
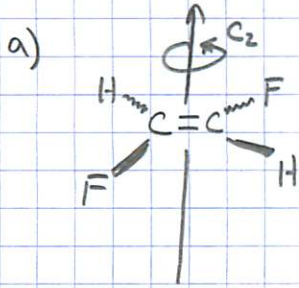
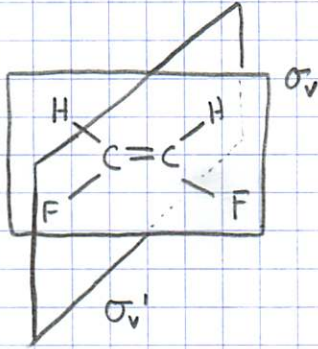
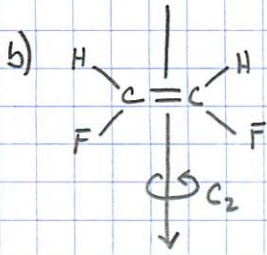


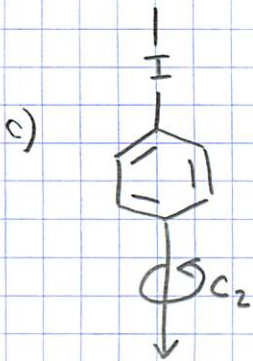
i) All molecules possess  $E$  + the symmetry elements highlighted below:



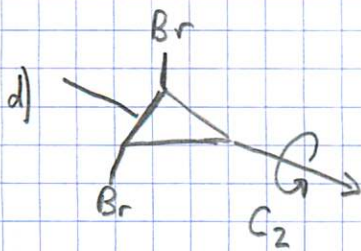
$C_2, \sigma_h, i$  ( $C_{2h}$ )  
Achiral



$C_2, \sigma_v, \sigma_v'$  ( $C_{2v}$ )  
Achiral



$C_2, \sigma_v, \sigma_v'$  ( $C_{2v}$ )  
Achiral



$C_2$  Chiral

2. Assign point groups for the following. For cases in which the structure is not drawn, assume the lowest energy conformation.

(a) HF  $C_{\infty v}$

(b)  $NH_3$   $C_{3v}$

(c) Toluene  $C_s$

(d)  $O=C=C=C=O$   $D_{\infty h}$

(e) cubane  $O_h$

(f)  $W(CO)_6$   $O_h$

(g) Benzene  $D_{6h}$

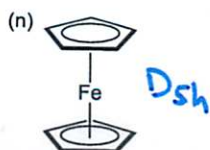
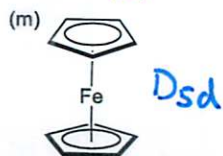
(h) adamantane  $T_d$

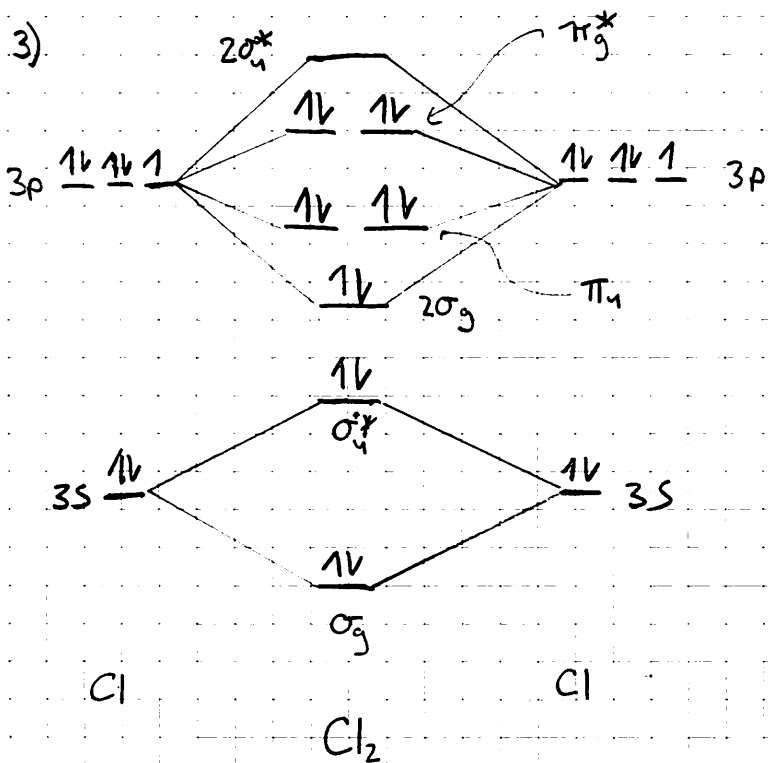
(i)  $P_4$   $T_d$

(j) Naphthalene  $D_{2h}$

(k)  $\pi$ -bond  $C_{2v}$

(l)  $\pi$ -antibond  $C_{2h}$

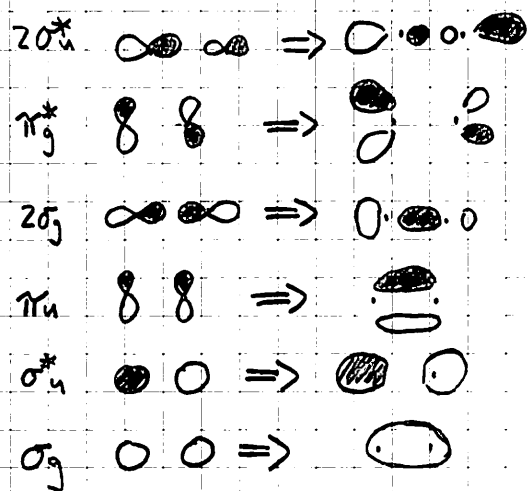
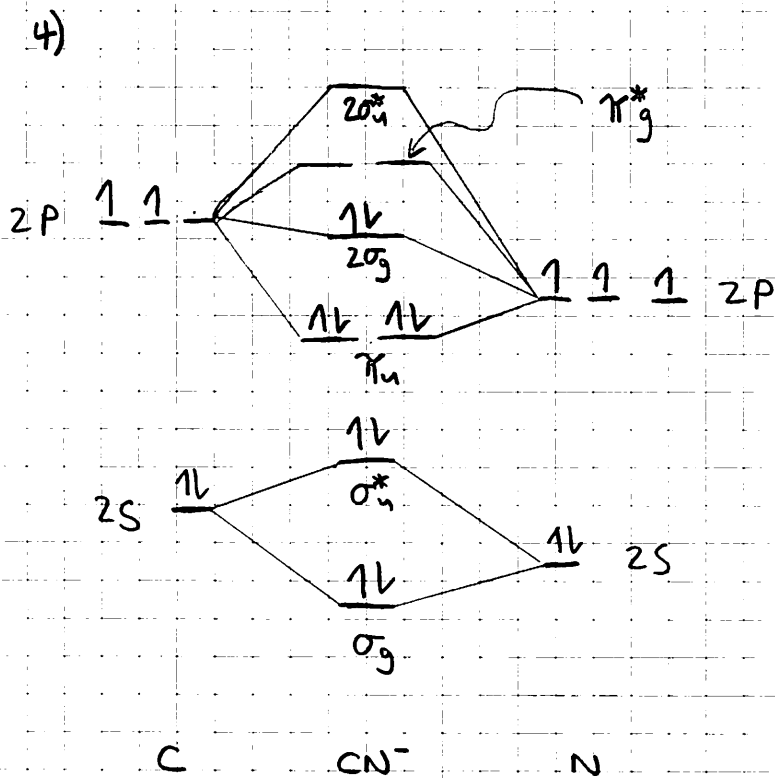




Cl<sub>2</sub> has 4 e<sup>-</sup> in the π\* MO + a bond order of 1

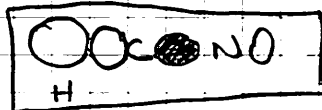
Cl<sub>2</sub><sup>+</sup> has 3 e<sup>-</sup> in the π\* MO + a BO of 1.5

Since the BO of Cl<sub>2</sub><sup>+</sup> is larger than the BO of Cl<sub>2</sub> the cation should have a shorter Cl-Cl bond length

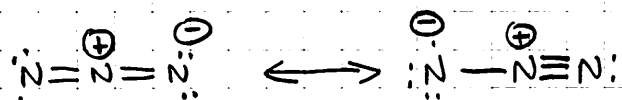


a) BO = 3 because π<sub>u</sub> + 2σ<sub>g</sub> are full while π<sub>g</sub><sup>\*</sup> + 2σ<sub>u</sub><sup>\*</sup> are empty.

b) FMO Theory suggests that the HOMO of CO will interact w/ the LUMO of the Lewis acid (H<sup>+</sup>). ∴ 2σ<sub>g</sub> of CO will interact with the empty 1s orbital of a proton



5)



- VSEPR suggests  $\text{N}_3$  will be linear
- For the representative above, the central N is linearly coordinated + has 2  $\pi$ -bonds consistent w/ sp hybridization
- Overall the bonding (By VBT) shows  $4 \times \sigma e^- + 4 \times \pi e^-$
- There is one unpaired  $e^-$   $\therefore \text{N}_3$  is a doublet
- Based on the 2 resonance structures,  $\text{N}_3$  is nonpolar
- The bond length of  $\text{N}_2$  is shorter than  $\text{N}_3$  since the  $\text{N}=\text{N}$  bonds for  $\text{N}_3$  have double bond character, + the  $\text{N}\equiv\text{N}$  bond of  $\text{N}_2$  is a triple bond

6)

X-Ray Diffraction - Bond Lengths + Angles

XANES - Oxidation State, geometry + coordination environment

Microwave Spectroscopy - Bond Lengths + Angles

IR Spectroscopy - Bond strength + functional group analysis