Practice sheet #6: Molecular Shape, Hybridization, Molecular Orbitals.

1. Draw the 3D structures for the following molecules. You can omit the lone pairs on peripheral atoms, but you need to show those on the central atom.

BF_3

NO_2^-

SO_2

$SeCl_2F_2$

2. For each of the molecules from problem 1, write the VSEPR formula:

BF_3 _____ **NO_2^-** _____

SO_2 _____ **$SeCl_2F_2$** _____

3. On each of the molecules of problem 1, draw the bond dipole and say whether the overall molecule is polar or not.

BF_3 _____ **NO_2^-** _____

SO_2 _____ **$SeCl_2F_2$** _____

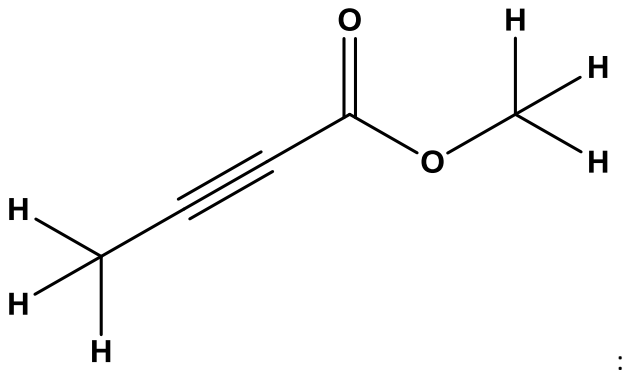
4. Looking at the molecules in problem 1, say what is the bond angle between the following atoms. Note: you need to account for distortions; i.e.: when an angle is not the expected value, write "less than/more than".

F-B-F _____ **O-N-O** _____

O-S-O _____ **Cl-Se-Cl** _____

Cl-Se-F _____ **F-Se-F** _____

5. Assign the hybridization state to every non-hydrogen atom of the following molecule



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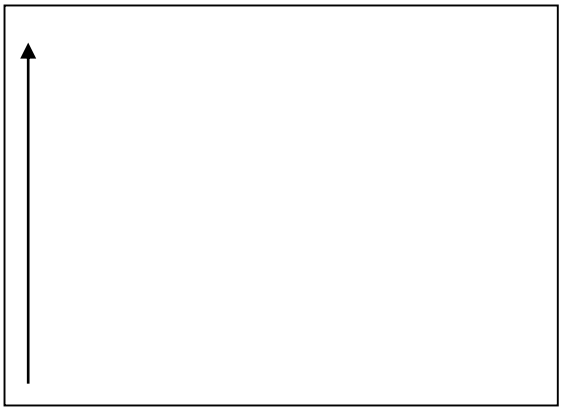
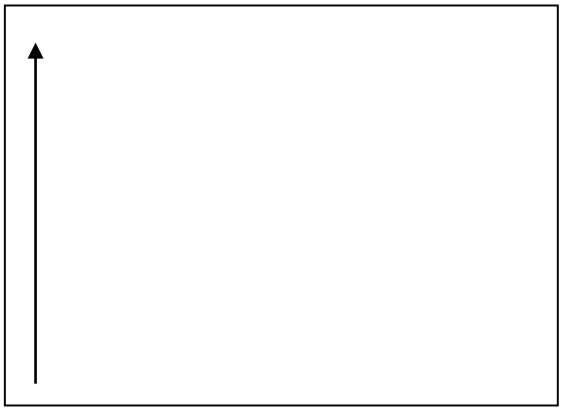
6. Sketch the molecular orbitals for the molecule in problem 5.

7. Draw the energy diagrams for the MOs of He_2 and He_2^+.

He_2



He_2^+



8. Which of the two species in question 7 has a higher bond order?

9. Comprehensive problem to wrap up this first half of the semester: A compound has an elemental % composition of H = 2.14; N = 29.79; O = 68.06 and its molar mass was found to be 47 g/mol. Sketch its molecular orbitals.

10. Diatomic heteronuclear molecule SO.
    - Draw the molecular orbital for SO (Sulfur Oxide) using NON-hybrid orbitals.

    - Write its electronic configuration:

      _____

    - What will the bond order between Oxygen and Sulfur be in Sulfur Oxide? _____

- Draw the Lewis structure for SO and assign the hybridization to each atom.

- Draw the molecular orbital for SO (Sulfur Oxide) using hybrid orbitals.

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- Sketch the MO for the molecule of SO.

- For each orbital of the MO drawn in part e, sketch the relative atomic orbital overlap.

11. Polyatomic molecule CO_2.
    - Draw the Lewis structure of CO_2 and assign the hybridization to every atom.

    - Sketch the molecular orbitals for CO_2

    - Using hybrid atomic orbitals, draw the MO's energy diagram for CO_2 (Hint: put carbon on the left side and both oxygen atoms together on the right side)

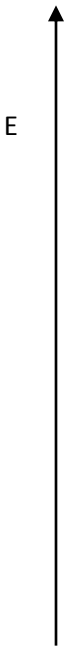
E

    - Right the electron configuration for the MO of CO_2

12. Dimeric polyatomic molecule N_2H_4.
    - Draw the Lewis structure of N_2H_4 and assign the hybridization to every atom.

    - Sketch the molecular orbitals for N_2H_4

    - Using hybrid atomic orbitals, draw the MO's energy diagram for N_2H_4 (Hint: put the two nitrogen atoms on the left side and the four hydrogen atoms, all together on the right side)



    - Right the electron configuration for the MO of N_2H_4

13. Butadiene is a hydrocarbon, which has a structure with two double bonds conjugated to each other; the condensed formula is CH_2-CH-CH-CH_2.
    - Draw the Lewis structure for butadiene.

    - Since all carbon atoms are sp^2 hybridized, the whole molecule is planar. Looking at it from the "side", it can be drawn omitting the hydrogen atoms and the σ framework, in order to display only the conjugated π system. Draw the MO's which form such conjugated π system. Order them by energy.

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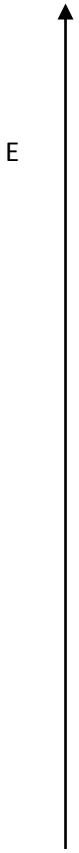
    - Label each of the molecular conjugated π systems drawn in part b as Ψ_I, where I is an integer increasing number (1 is for the wave-function lowest in energy, then 2, 3, 4, etc…. as many as needed).

    - Fill the Ψ_I in part b in, with the appropriate number of electrons.

    - Label the Ψ_I in part b as bonding, non-bonding, anti-bonding (π, n, π^*).

14. Nitrogen dioxide (NO_2) is a poisonous gas which has a structure with a double bond and a conjugated lone pair.
    - Draw the Lewis structure for nitrogen dioxide.

    - Since all atoms are sp^2 hybridized, the whole molecule is planar. Looking at it from the "side", it can be drawn omitting the σ framework (including the lone pairs contained in σ orbitals), in order to display only the conjugated π system. Draw the MO's which form such conjugated π system. Order them by energy.



    - Label each of the molecular conjugated π systems drawn in part b as Ψ_I, where I is an integer increasing number (1 is for the wave-function lowest in energy, then 2, 3, 4, etc…. as many as needed).

    - Fill the Ψ_I in part b in, with the appropriate number of electrons.

15. Label the Ψ_I in part b as bonding, non-bonding, anti-bonding (π, n, π^*).