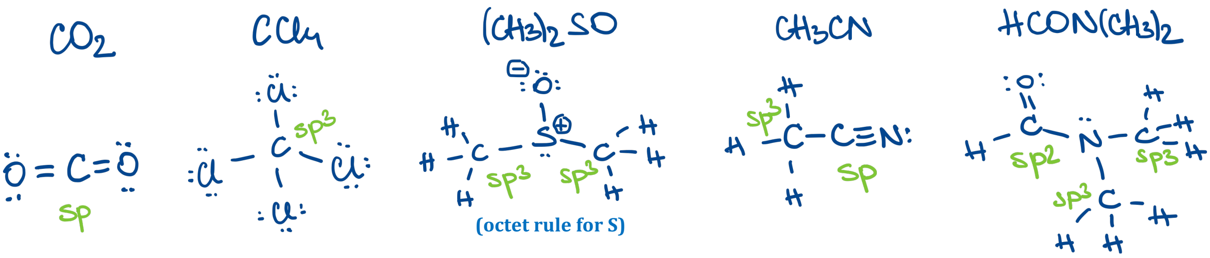
Organic Chemistry - Exercise 2

Distribution: October 3 2025

Help: October 9 2025

Return until: October 11 2025

1. For each of the following compounds, draw their Lewis structures (please explicitly draw all lone pairs) and give the hybridization of each carbon atom in their structure.
    a. carbon-dioxide (CO_2)
    b. carbon tetrachloride (CCl_4)
    c. dimethyl sulfoxide ($(CH_3)_2S{=}O$)
    d. acetonitrile (CH_3CN)
    e. *N,N*-dimethyl formamide ($H(C{=}O)N(CH_3)_2$)



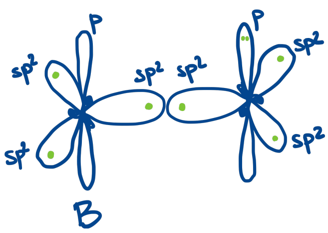
2. This exercise is about aminoborane $(CH_3)_2B{-}N(CH_3)_2$.
    a. According to VSEPR theory, which hybridization states are expected for boron and nitrogen in this compound?

       Since boron atom is bonded to two methyl groups and a nitrogen atom, it is expected to have sp^2 hybridization. Nitrogen atom is bonded to two methyl groups and a boron atom, and also has a lone electron pair, so the expected hybridization is sp^3.

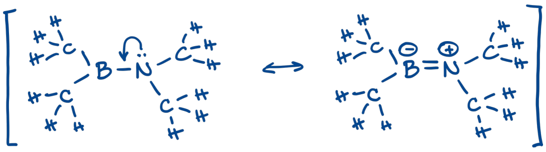
    b. It is experimentally shown that *both* boron and nitrogen atoms have a trigonal-planar coordination geometry. What are then the *real* hybridization states of these two atoms in this compound?

       As both atoms are in trigonal-planar surroundings, both their hybridizations have to be sp^2. The lone pair of nitrogen atom is located in a non-hybridized 2p orbital.

    c. After the conclusions in the previous task, draw Valence Bond model of this compound (focus only on B and N atoms).



d. Draw two Lewis resonance structures of this molecule. What is the expected bond order of the B–N bond approximately? What is the expected orientation of the dipole moment if this molecule and why?



The expected bond order is 1.5 (between 1 and 2).

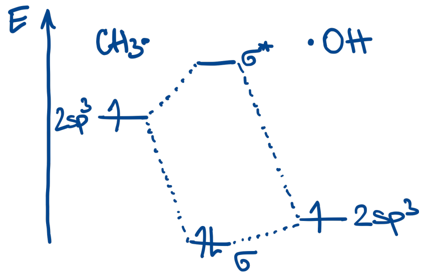
Nitrogen has a negative inductive effect due to higher electronegativity than boron, but it has a positive mesomeric effect, since its lone pair can interact with empty p orbital of boron. As the mesomeric effect is stronger, the negative pole will be on the boron atom and the positive pole will be on the nitrogen atom.

3. This exercise is about bond formation in methanol (CH_3OH).

a. According to VSEPR theory, what are the hybridizations of carbon and oxygen atoms in methanol and why?

The carbon atom in methanol is bonded to three hydrogen atoms and an oxygen atom, so its hybridization is sp^3. The oxygen atom is bonded to one carbon and one hydrogen atom and additionally has two lone pairs, so its hybridization is also sp^3.

b. Draw the MO diagram of methanol by showing the bonding between $H_3C\cdot$ and $\cdot OH$ fragments.

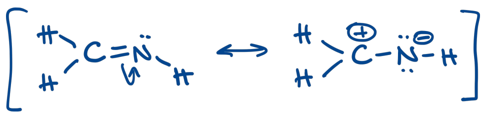


c. Does the bonding molecular orbital look more like the orbital of oxygen or the one of carbon and why?

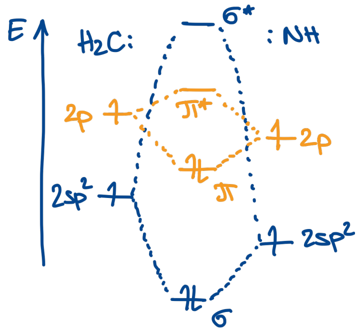
The bonding orbital looks more similar to oxygen orbital, since it is more electronegative than carbon.

4. This question is regarding the bond formation in methanimine ($H_2C{=}NH$).

a. Draw two resonance structures of methanimine indicating all lone pairs.



b. Draw the MO diagram of methanimine showing the bond formation between H_2C: and :NH fragments.



c. Why does 2p orbital of carbon atom does not interact with $2sp^2$ orbital of nitrogen atom?

Only orbitals with matching symmetry and orientation can interact with each other – p orbitals with p orbitals and sp^2 orbitals with sp^2 orbitals of the right orientation.

d. Why is the energy difference between formed π and π^* orbitals smaller than the energy difference between formed σ and σ^* orbitals?

σ bond is obtained by end-on overlapping of atomic orbitals (pointing to each other), while π bonds are obtained by side-on overlapping of atomic p orbitals. As the interaction is much stronger in case of end-on overlapping, the energy splitting is higher in the case of σ bond formation.

Reading Suggestions:

Clayden, Greeves, Warren, Wothers, *Oxford University Press*, **2001**.

Organic Chemistry, John McMurry, *Thomson Brooks/Cole*, **2008**.

Chimie Organique, Les Grands Principes, John McMurry, *Dunod Editeur*, **2009**.

Chimie Organique, Paul Arnaud, *Dunod Editeur*, **2009**.