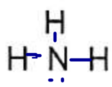
Worksheet – Hybridization #1

One model to explain bonding in molecules is called the **valence bond theory**. It is based on the concept of **hybridized molecular orbitals.** Atomic orbitals (*s,p,d*) are mathematically mixed to form molecular orbitals with defined shapes and energy levels. In organic chemistry, we need only look at the hybridization of the one 2*s* and three 2*p* orbitals containing the valence electrons of C,O and N.

When **four** equivalent molecular orbitals are needed, all **four** atomic orbitals are mixed to give ***sp*^{3} hybridization.** When **three** equivalent molecular orbitals are needed, **three** of the atomic orbitals are mixed to give ***sp*^{2} hybridization.** In this case, one unhybridized ***p*** atomic orbital remains, with its shape and energy level unchanged. When **two** equivalent molecular orbitals are needed, only **two** of the four atomic orbitals are mixed, giving ***sp* hybridization.** Two unhybridized atomic *p* orbitals remain.

1. Lewis structures help to determine how many equivalent molecular orbitals are present. Complete the Lewis structure of ammonia, NH_3.



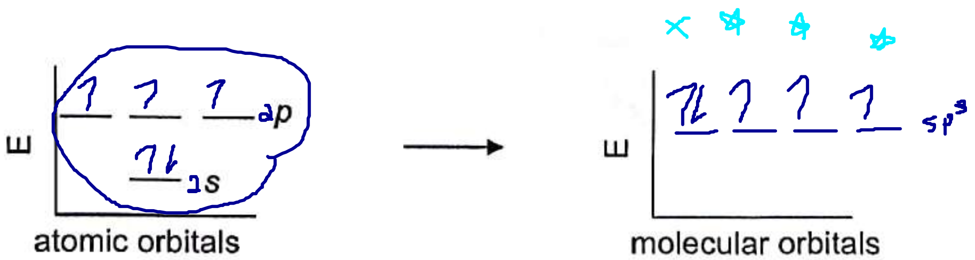
   a. How many atoms are bonded to N ___3___

   b. How many lone pairs of e$^-$ are on N ___1___ 3

   c. How many equivalent molecular orbitals ___4___ steric #

   d. Hybridization ___sp^3___

   e. Fill in the e$^-$ for atomic N
   f. Draw the hybrid orbitals for NH_3
   g. Fill in the e$^-$ for N in NH_3
   h. Compare the Lewis structure with the molecular orbital diagram



2. Complete the Lewis structure of carbon dioxide, CO_2.

$$:\ddot{O}=C=\ddot{O}:$$

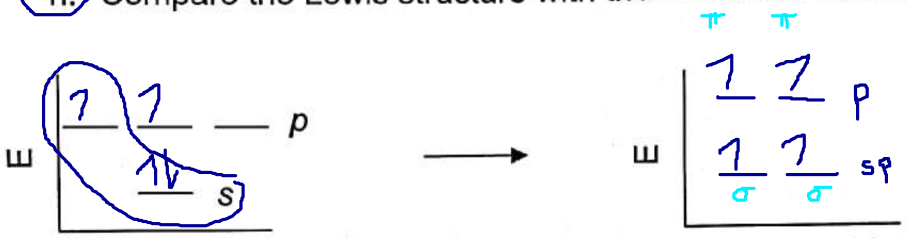
a. How many atoms are bonded to C 2

b. How many lone pairs of e⁻ are on C + 0

c. How many equivalent molecular orbitals 2

d. Hybridization sp

e. Fill in the e⁻ for atomic C
f. Draw the hybrid orbitals for C in CO_2
g. Fill in the e⁻ for C in CO_2
h. Compare the Lewis structure with the molecular orbital diagram



atomic orbitals   molecular orbitals

3. Repeat this for the oxygen in CO_2.

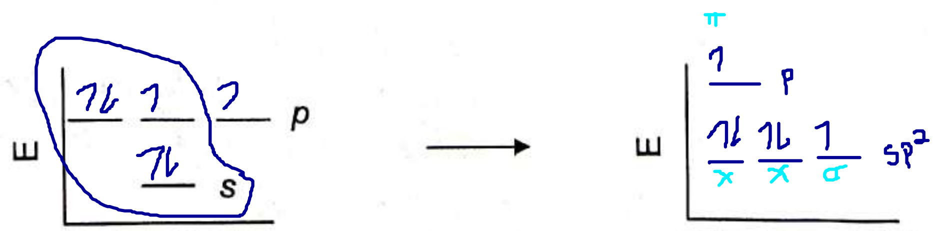
a. How many atoms are bonded to O 1

b. How many lone pairs of e⁻ are on O + 2

c. How many equivalent molecular orbitals 3

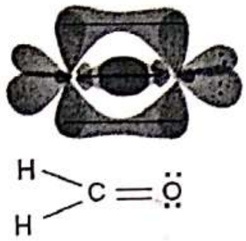
d. Hybridization sp^2

e. Fill in the e⁻ for atomic O
f. Draw the hybrid orbitals for O in CO_2
g. Fill in the e⁻ for O in CO_2
h. Compare the Lewis structure with the molecular orbital diagram

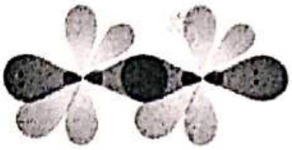


atomic orbitals   molecular orbitals

Bonds made with hybridized orbitals are called σ (sigma) bonds. All single bonds are σ-bonds. Bonds made with unhybridized *p* orbitals are called π (pi) bonds. In multiple bonds (= or ≡) one bond is a σ-bond and the others are π-bonds. Sigma bonds result from the end-to-end overlap of hybridized orbitals. The bonding electrons are held directly between the two nuclei. Pi bonds result from the side-to-side overlap of *p* orbitals. The bonding electrons are held above and below the two nuclei.



The top figure shows the electronic structure of CH_2O. The C and O are both sp^2 hybridized. Two of the orbitals on O are populated with lone pair e^-. The bond angle between the hybridized orbitals is **120°** making this a **trigonal planar** structure. The unhybridized *p* orbital is at 90° to the sp^2 orbitals

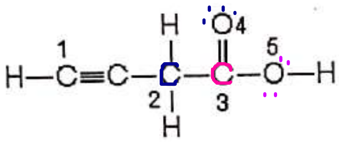


:N≡N:

The bottom figure shows the electronic structure of N_2. Both N are *sp* hybridized, with **180°** between these orbitals. One hybridized orbital forms a σ-bond and a lone pair of e^- occupies the other. The two *p* orbitals on each N form two π bonds between the atoms.

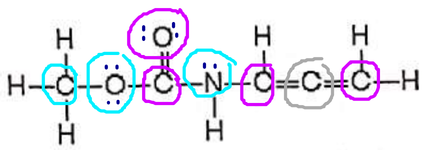
The four sp^3 orbitals lie at **109.5°** to each other and form a **tetrahedron**.

4. For the compound below, determine the hybridization, bond angles and lone pair e^- at each numbered atom.



	hybridization	bond angle	lone pair e^-
1	sp	180°	0
2	sp^3	109.5°	0
3	sp^2	120°	0
4	sp^2	120°	2
5	sp^3	109.5°	2

5. For the compound below determine



a. How many sp^3, sp^2 and *sp* hybridized atoms are present 3 4

b. How many lone pairs of e^- are present 5

c. How many σ-bonds are present 14

d. How many π-bonds are present 3

Scanned with CamScanner

It is often possible to draw more than one Lewis structure for a compound. For example, N_2O can be drawn as:

: N : N : : : O :   N : : N : : O   : N : : : N : O :

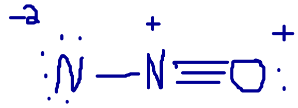
To determine which structure is the most reasonable, the **formal charge** on each of the atoms in the molecules can determined. The formal charge is an indication of the electron density at the atoms in a particular structure. It is determined as:

formal charge = valence e^- - lone pair e^- - ½ shared e^-

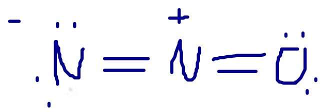
Nitrogen is in Group V, and has 5 valence electrons. Oxygen is in Group VI, with 6 valence electrons.

6. Assign formal charges to all of the atoms in the three resonance structures of N_2O.

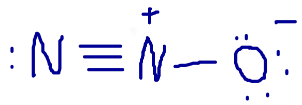
a. : N : N : : : O :



b. N : : N : : O



c. : N : : : N : O :



d. Based on the chemical nature of these elements, which is the worst structure and why?

a - charge sep.

e. Which is the best structure, and why?

c- neg charge on most electronegative atom

The atomic Lewis structures of C, N and O are · C · · N · · O ·

7. What is the most stable bonding pattern for

	bonds	lone pair e^-
a. C	4	0
b. N	3	1
c. O	2	2