Hybrid Theory

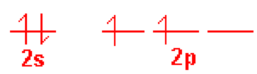
1. What orbitals are available for bonding for each atom involved in the molecule?

Each hydrogen has a 1s orbital available for bonding.
Carbon has one 2s and 3 2p orbitals available for bonding.

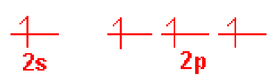
This was determined by looking at the valence of each atom. Rememebr that only valence electrons participate in bonding.

2. Based on this would you expect all the C-H bonds in methane (CH_4) to be identical?

To answer this let's look at the valence electron configuration for carbon.

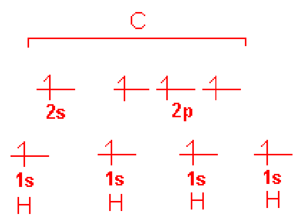


In it's current format, it doesn't look like carbon can make more than 2 bonds, as it has only 2 unpaired electrons. What winds up happening is that one of the 2s electrons gets promoted into the 2p shell so that we get:

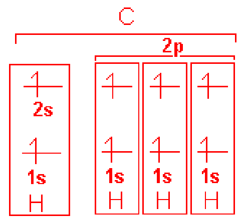


When this happens, we are now able to bond carbon 4 times, as there are four unpaired electrons.

Next let's consider this in conjunction with the 4 hydrogen atoms.



From this we can see that each one of the hydrogens can pair up with one of the unpaired electrons from the carbon atom.



Looking at these results we can now say that based on this initial information we would expect 3 of the four bond to be identical. This is the case because 3 of the bonds are made from a 1s/2p combination and one bond is made from a 1s/2s combination. Different orbitals used = different bonds.

3. What have experiments shown?

Experiments have shown that all bonds are actually equivalent (i.e. identical to one another)..

4. What does this indicate?

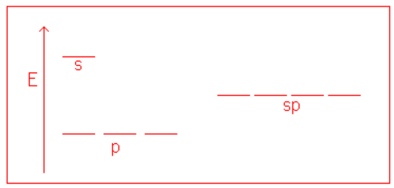
This means that carbon cannot be using its atomic orbitals (2s and 2p). If all bonds are identical is must be using 4 equivalent orbitals to bond with the hydrogens.

5. This means that when an atom patricpiates in a bond, its atomic orbitals (regular valence shell orbitals) are combined to form a hybrid. This new

hybrid orbital is what particpates in the bond.

6. How does the energy of the hybrids compare to the atomic orbitals?

The hybrid orbital has an energy level somewhere between the energy level of the composite atomic orbitals.



7. The number of hybrid orbitals formed is equal to the number of atomic orbitals used.

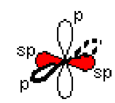
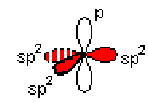
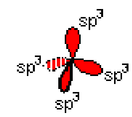
8. What should you do first, when trying to determine the type of hybrid orbitals needed?

Draw out your Lewis Dot structure.

a. Why?
It will help you to determine the number of areas of electron density (or steric number) of each of atom in the molecule. The type of hybrid used depends on the steric number.

b. How many areas of electron density do the following account for?
    i. Lone Pairs - one
    ii. Single bond - one
    iii. Double Bond - one
    iv. Triple Bond – one

9. Fill In the Following

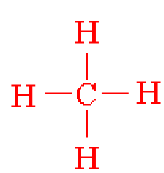
Orbital Mixing Ratio			Result	Areas of Electron density	Drawn	Shape
s	p	-	2sp hybrid orbitals + 2 unhybridized p orbitals	2		Linear
s	2p	-	3sp^2 hybrid orbitals + 1 unhybridized p orbital	3		Trigonal Planar
s	3p	-	4sp^3 hybrid orbitals	4		Tetrahedral
s	3p	d	5sp^3d hybrid orbitals + 4 unhybridized d orbitals	5	-	Trigonal Bipyramidal
s	3p	2d	6 sp^3d^2 hybrid orbitals + 3 unhybridized d orbitals	6	-	Octahedral

*hybrids are in red

10. Draw the following

a. CH_4

Step 1 – Lewis Dot



Step 2 – Determine the Steric Number for Atoms in Molecule

Carbon

Steric Number = 4

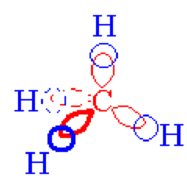
This means we will need to create a hybrid that has 4 orbitals.

This means we need to combine 4 atomic orbitals. One s and three p orbitals – which come together to form 4sp^3 hybrids.

Hydrogen

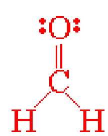
doesn't create hybrid orbitals because it only has a 1s electron available

Thus, the molecule would look like:



b. CH_2O

<u>Step 1 – Lewis Dot</u>



<u>Step 2 – Determine the Steric Number for Atoms in Molecule</u>

Carbon

Steric Number = 3

This means that we need to create 3 hybrid orbitals.

So we need to combine 3 atomic orbitals. One s and two p orbitals – which come together to form 3 sp^2 hybrids and one unhybridized p is left over.

Oxygen

Steric Number = 3

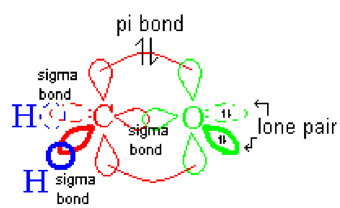
This means that we need to create 3 hybrid orbitals.

This means we need to combine 3 atomic orbitals. One s and two p orbitals – which come together to form 3 sp^2 hybrids and one unhybridized p is left over.

Hydrogen

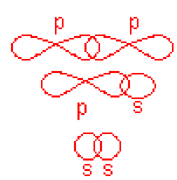
Does not form hybrids

Thus the molecule would look like:



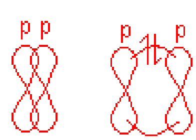
11. What are sigma and pi bonds?

Sigma bonds are bonds that occur when orbitals have a head on overlap.



These are all examples of sigma bonds.

Pi bonds overlapping parallel p orbitals.



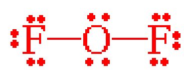
These are two ways to represent the pi bond.

12. What are each type of bond composed of?

Single = 1 sigma bond
Double = 1 sigma bond + 1 pi bond
Triple = 1 sigma bond + 2 pi bonds

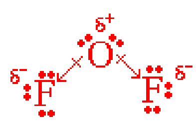
13. Predict the shape, hybridization of central atom and polarity for the following

a. OF_2

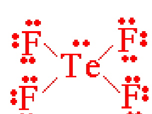


Shape – Bent (4 areas of e^- density and 2 lone pairs)
sp^3 hybridization (Steric Number = 4, combination of 4 atomic orbitals).

Polar

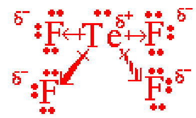


b. TeF_4

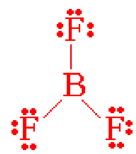


Shape – See Saw (5 areas of e^- density and 1 lone pair)
sp^3d hybridization (Steric Number = 5, combination of 5 atomic orbitals)

Polar



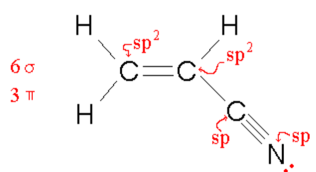
c. BF_3

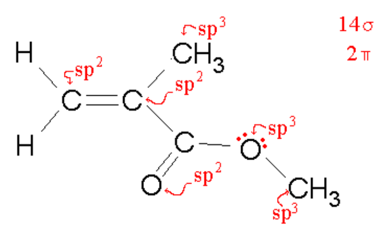


Shape – Trigonal Planar (3 areas of e^- density)
sp^2 hybridization (Steric Number = 3, combination of 3 atomic orbitals)

Non-polar (symmetry cancels out polar bonds)

14. Label the hybridization of C, O, and N in the following molecules. Also count total number of sigma bonds and total number of pi bonds.





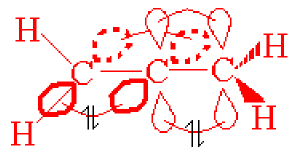
15. Are all the atoms in the same plane?

a. C_2H_2

$$H-C\equiv C-H$$

This would be a linear molecule (2 areas of e^- density around each carbon, no lone pairs)

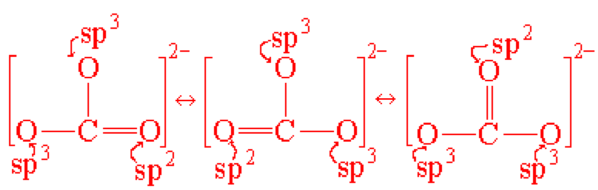
b. CH_2CCH_2



All of the atoms are not in the same plane. In order for the central carbon to double bond to each of the outer carbons they must form a pi bond. Pi bonds are made up of parallel p orbitals. This means that one of the carbons will have to bond with the p_y and the other will bond with the p_x. The sigma bonds occur on the z plan.

16. How can CO_3^{2-} help us understand the short falls of LE model?

If you look at the Lewis Dot for CO_3^{2-}:



This is a resonance structure. As you can see based on where we position the double bond, the hybridization of the oxygen atoms change. We cannot label it sp^2 or sp^3. Our model is falling short here because we cannot describe resonance structures. This means that we need to revise our understanding a bit.