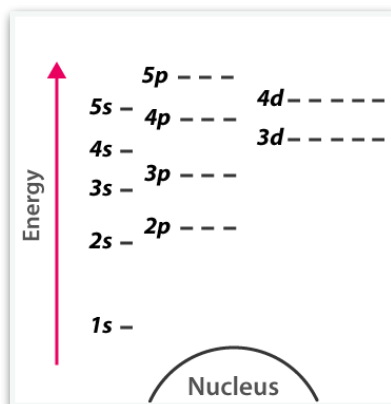


# Covalent Bonds

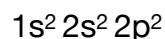
## Molecular Orbitals

- Electrons that are the farthest away from the nucleus are called valance electrons. All the other electrons in an atom called core electrons.
- If we take the valance electrons from the electron configuration those are the electrons that can participate in covalent bonding, which is the sharing of electrons, because they are on the outer portion of the atom that are able to interact with other atoms.
- Before valance electrons can form a covalent bond they must go through a promotion and hybridization phase so that the energy levels of each electron that has potential to form a bond will be equal. Each orbital has a different amount of energy associated with it as shown:



- Consider the electron configuration of carbon and hydrogen.

**Carbon:**

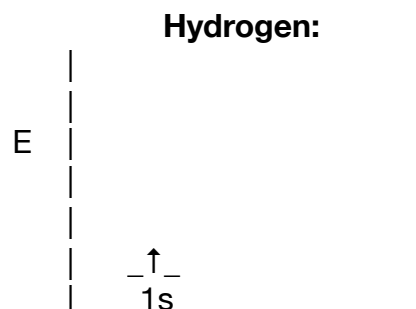
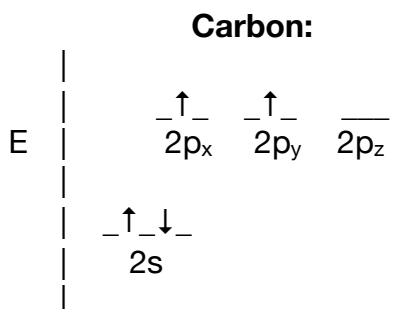


**Hydrogen:**



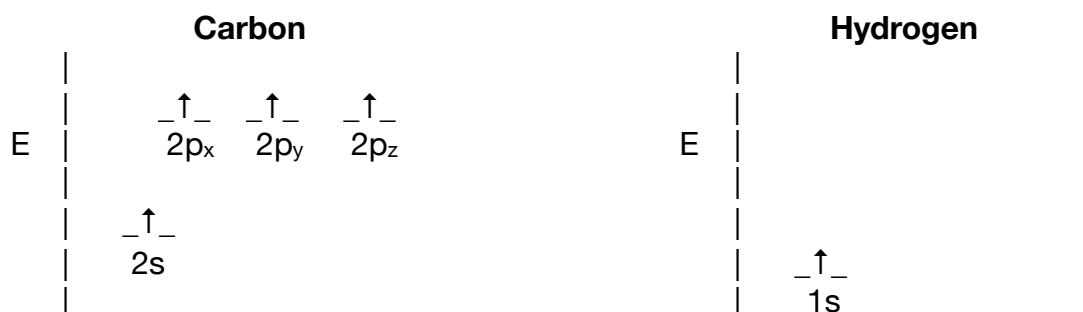
- The valance electrons for carbon are  $2s^2 2p^2$  and the valance electron for hydrogen is  $1s^1$ . Now we will make an energy diagram for each atom.

### Electron Configuration:



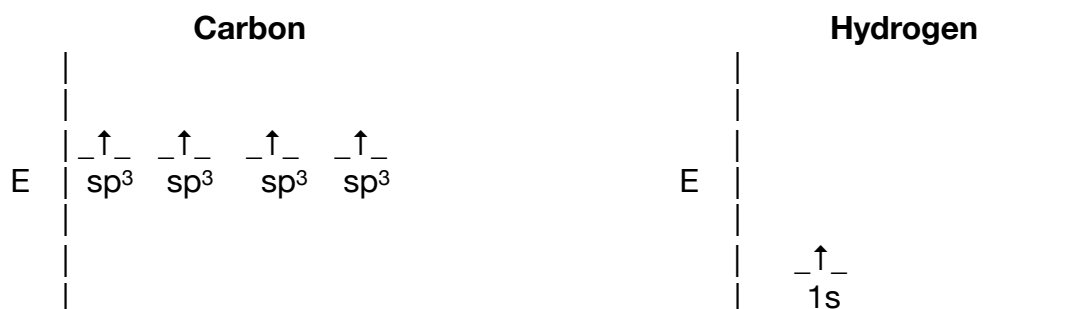
- Before bonds can be made the electrons in the diagram above need to go through a promotion phase so that each valence electron is spaced out into different orbitals as much as possible to prepare for bonding so that an additional electron (the one that is being shared) can occupy any of the available orbitals.

### Promotion Phase:

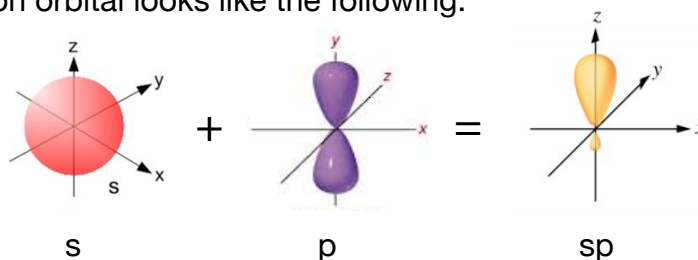


- The electron that gets promoted in this stage is called **excited** because energy was put in to bring it to a higher energy level. Before the electron got excited it was at its **ground state**. After the promotion phase the electrons go through a hybridization phase.

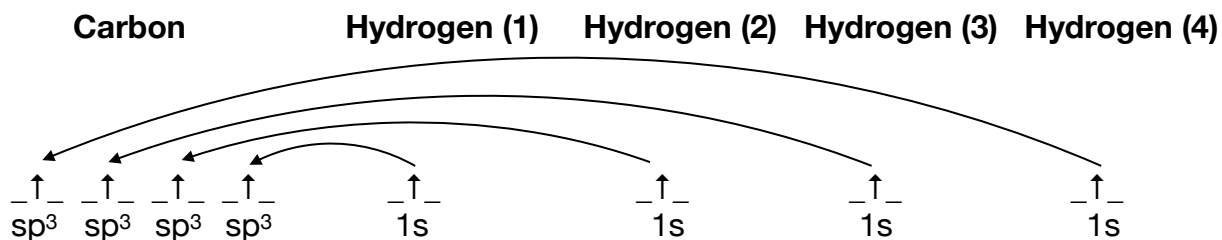
### Hybridization Phase:



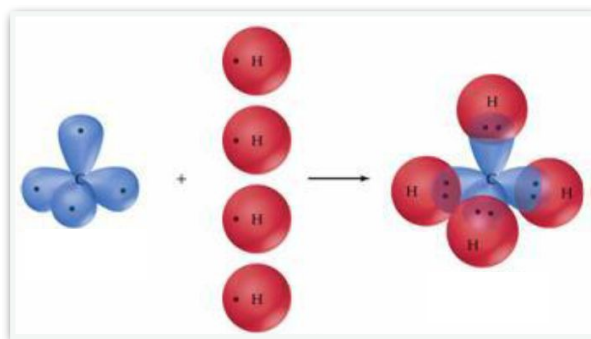
- Notice that the hydrogen did not go through a promotion or hybridization phase. That is because it only has one electron.
- The reason the carbon hybridization orbitals are called  $sp^3$  is because they were made from one s orbital and three p orbitals (1 s orbital plus 3 p orbitals makes a  $sp^3$ ). A hybridization orbital looks like the following:



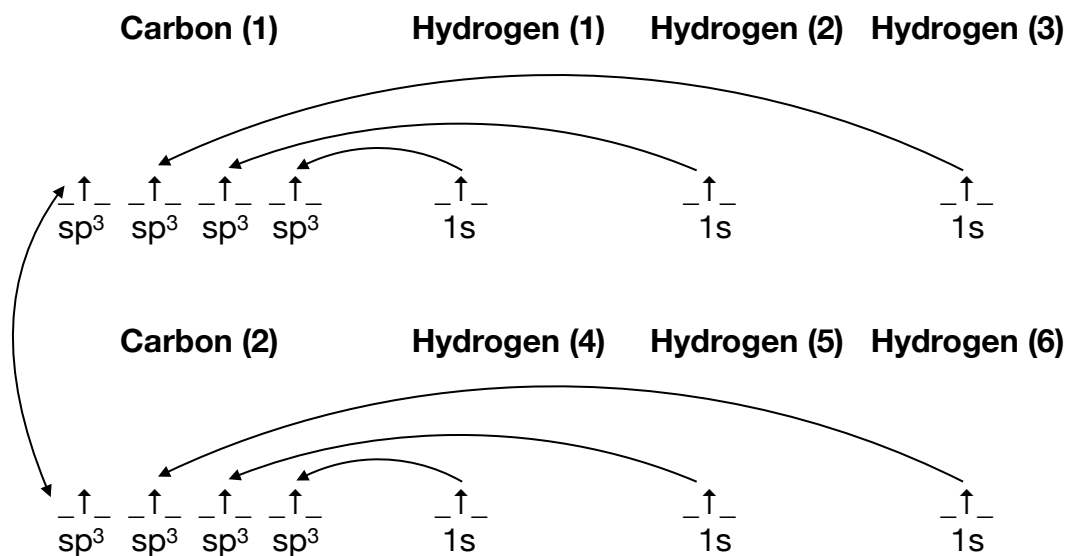
- Now that we have the hybridization for carbon we can draw out the lewis structure for a molecule like  $\text{CH}_4$ . In  $\text{CH}_4$  there is one carbon and four hydrogens, so we will write out the carbon and hydrogen hybridization orbitals.



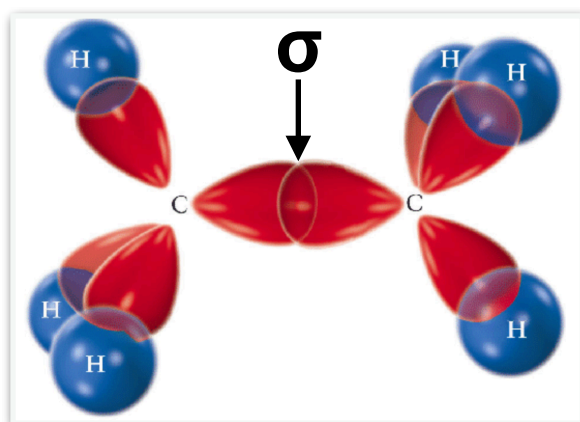
- Each arrow represents a bond of sharing electrons. If each orbital shares an electron in this way, then each orbital will have 2 electrons, which is what you want to have for the orbital to be considered full. A 3D figure of this molecule would look like this:



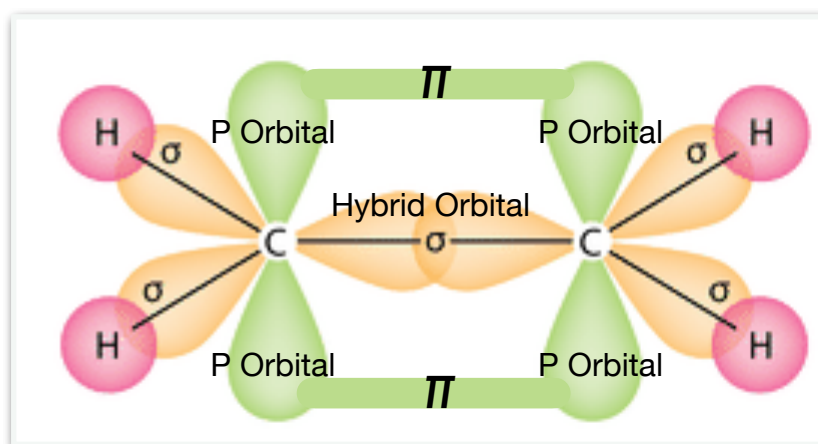
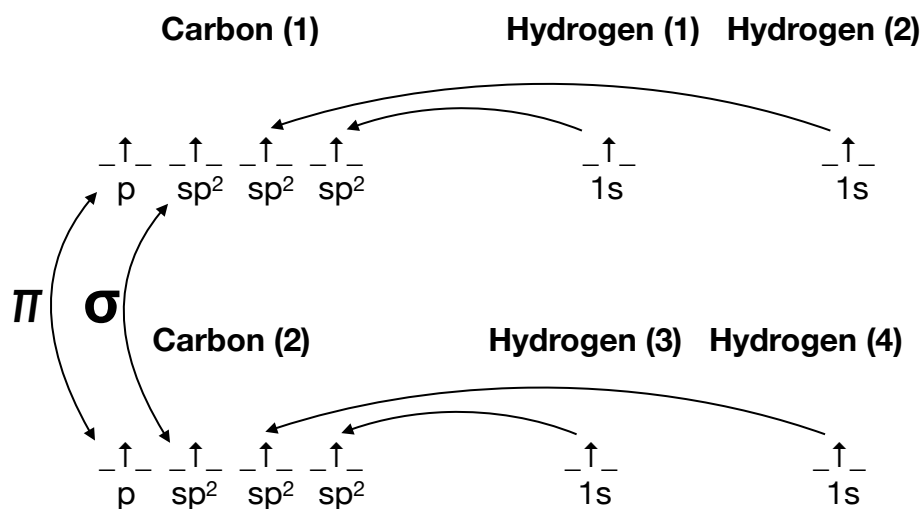
- Now let's do the same thing for  $\text{C}_2\text{H}_6$ . The hybridization for carbon and hydrogen are shown below:



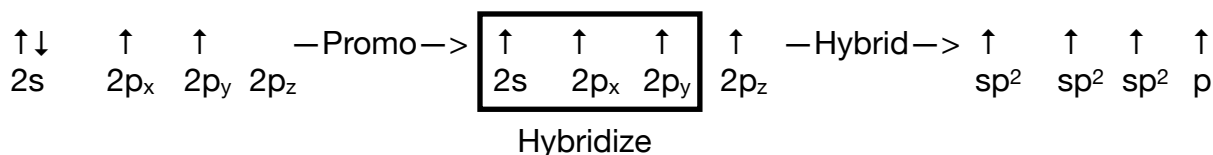
- If each arrow represents a covalent bond a 3D figure of this would look like the following. The overlap between the carbon-carbon bond is called a sigma bond.



- Each red orbital above represents a hybridized orbital. When carbon has 4 hybridized orbitals each orbital is called  $sp^3$  hybridized. Now let's do the same thing for  $C_2H_3$ .



- In order to bond all of the electrons in  $C_2H_6$  there must be two bonds between carbon and carbon. When two bonds form between two of the same atoms it is called a double bond. However, the second bond that forms between carbon and carbon is not a sigma bond, it is a pi bond. A pi bond is the bond between two p orbitals and a sigma bond is the bond between two hybrid bonds. After a sigma bond forms there is not enough room for another sigma bond to form so the second bond must go above and below the sigma bond. For a bond to go above and below a sigma bond the orbital can not hybridize and must be left as a p orbital. This means that when carbon goes through a hybridization phase only 3 of the 4 orbitals hybridize, which means the hybrid orbitals are the result of 1 s and 2 p so we use  $sp^2$  instead of  $sp^3$ .



- If a triple bond forms between two carbon atoms with each carbon also being bonded to a hydrogen it would be  $sp$  hybridize because it is made from 1 s and 1 p orbital.

**BEWARE:** Boron only has 3 valance electrons so  $BH_3$  forms it will be  $sp^2$  hybridized.

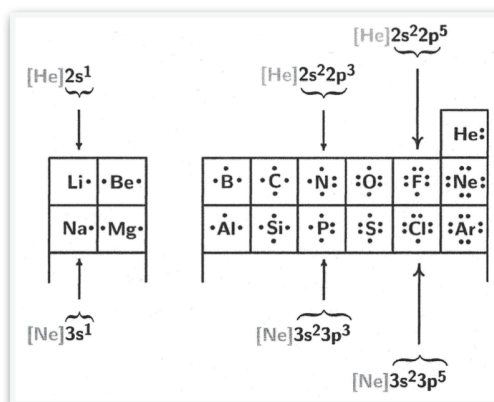
- If a chemical has a lone pair, like  $NH_3$ , the lone pair will occupy a hybridized orbital so  $NH_3$  will be  $sp^3$  hybridized.

## Lewis Dots

- When you are trying to figure out how to put the atoms together, instead of making up and down arrows, you can make lewis dots. Because there are 4 different orbitals per atom (the 4 orbitals come from the s and p - we will talk about d later) you put dots in a square shape around an atom where each side can only have 2 dots because there are only 2 electrons can fill an orbital. For example, N has 5 valance electrons so it gets 5 dots and looks like this:



- Because each column on the periodic table has the same number of valance electrons, each column will have the same number of lewis dots. The following picture show how lewis lots are made for the first 2 rows on the periodic table.



- Because each group on the periodic table has the same number of valence electrons chemicals in the same group will have similar reactivity. The different number of core electrons in each column has a minor effect on the chemical reactivity.

**BEWARE:** He only has 2 protons and 2 electrons. Those 2 electrons are the only valence electrons that it has not 8 like the noble gases.

- For now we will ignore the d orbital electrons and just focus on the s and p orbital electrons. If we add up the s and p electrons it will equal 8 electrons (2 from s and 6 from p). If the electrons in each orbital want to be filled, then each element wants to have 8 electrons, this is called the **octet** rule. If an atom does not have enough electrons to fill this octet it can share electrons with another element.
- Let's make a lewis structure for H<sub>2</sub>O. Oxygen has 6 valence electrons so it gets 6 dots. If oxygen gets 6 dots, then two of its four orbitals are full.



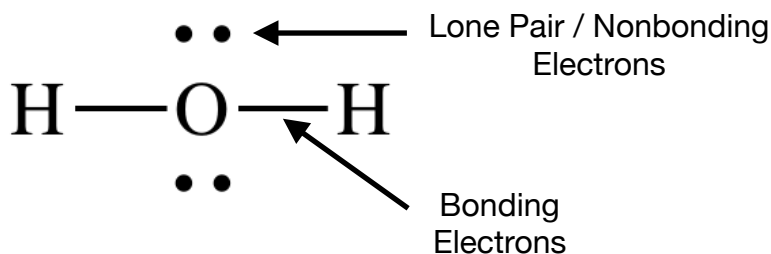
- H<sub>2</sub>O has two hydrogens and each hydrogen has only one orbital (not 4 like oxygen) that needs to be filled with two electrons, so it is an exception to the octet rule.



- Now we need to put all of the atoms together to form a molecule. If an atom at one dot on one side that represents an electron that is able to form a covalent bond.



- The circle represents a covalent bond and can be replaced with line. A double bond will have two lines and a triple bond will have three lines.



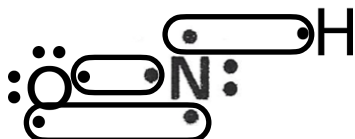
### Example-1

Make a lewis structure for NOH and N<sub>2</sub>. and determine the hybridization of all the atoms in the molecule.

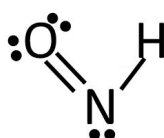
—First let's do NOH. Nitrogen has 5 valence electrons, oxygen has 6, and hydrogen has 1.—



—Now we can match up electrons that have one dot on one side.—



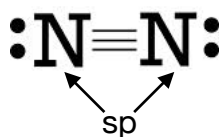
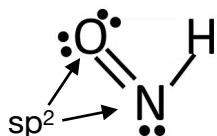
—Now replace the circles with bonds.—



—For N<sub>2</sub> we will do the same thing for two nitrogens.—

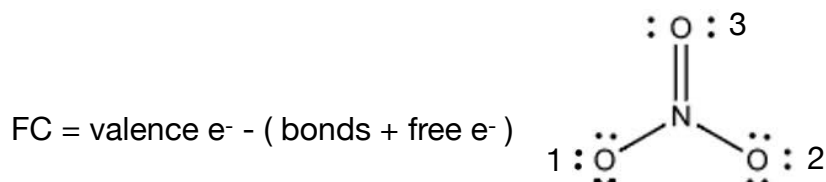


—The bond between the N and O in NOH has a double bond, which means one of them must be a sigma and the other is a pi. The triple bond between N and N in N<sub>2</sub> has a sigma bond and two pi bonds.—



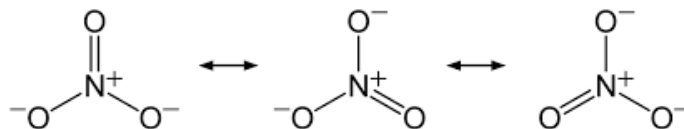
## Formal Charge and Resonance Structures

- Each atom in a Lewis structure has a formal charge. The formal charge of an atom is equal to the number of valence electrons that atom has minus the number of bonds plus the number of non bonding electrons. Consider the Lewis structure for NO<sub>3</sub><sup>-</sup>.



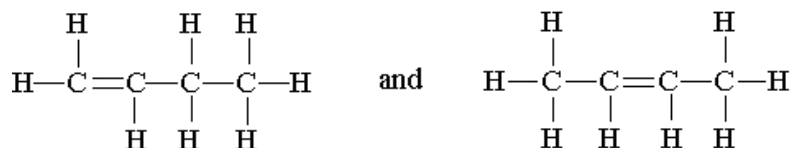
- The oxygen labeled 1 and 2 have a formal charge equal to -1 because  $6 - (1 + 6) = -1$ . The oxygen labeled 3 has a formal charge of +1 because  $5 - (4 + 0) = +1$ . This gives NO<sub>3</sub><sup>-</sup> an overall charge of -1 because  $(-1 + -1 + 1) = -1$ .

- When you form lewis structures with formal charges you always give as few charges as possible and have the most electronegative atom have the negative charge and the most electropositive atom have a positive charge.
- If you look at the structure for  $\text{NO}_3^-$  there is no reason why the double bond couldn't form between the first or second oxygen instead of the third oxygen. This creates a resonance structure as shown below where the actual structure of  $\text{NO}_3^-$  is a combination of all three structures.

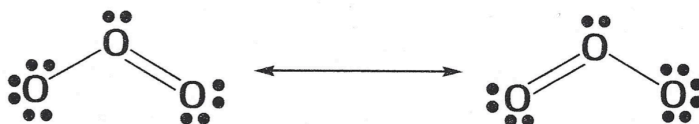


- When resonance structures form electrons are moving between two atoms and is a requirement for a resonance structure to form.

**BEWARE:** The following structures are not resonance structures. They are isomers.



- Another example of a resonance structure would be  $\text{O}_3$  because the arrangement of electrons is similar in both structures except that electrons are shifted to different atoms and the atoms themselves do not move.



## Molecular Geometry and Electron Domain Geometry

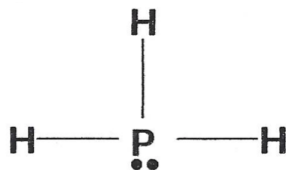
- The 2D molecules we have been drawing have a 3D shape. To determine the 3D shape of a molecule you have to determine how many domains a particular atom has. The atom you are counting the domains for will tell you the 3D shape around that particular atom.

### Example-2

How many domains are in the P atom in  $\text{PH}_3$  and how many of those are lone pairs.

—To determine the number of domains we first need to draw out the lewis structure.—



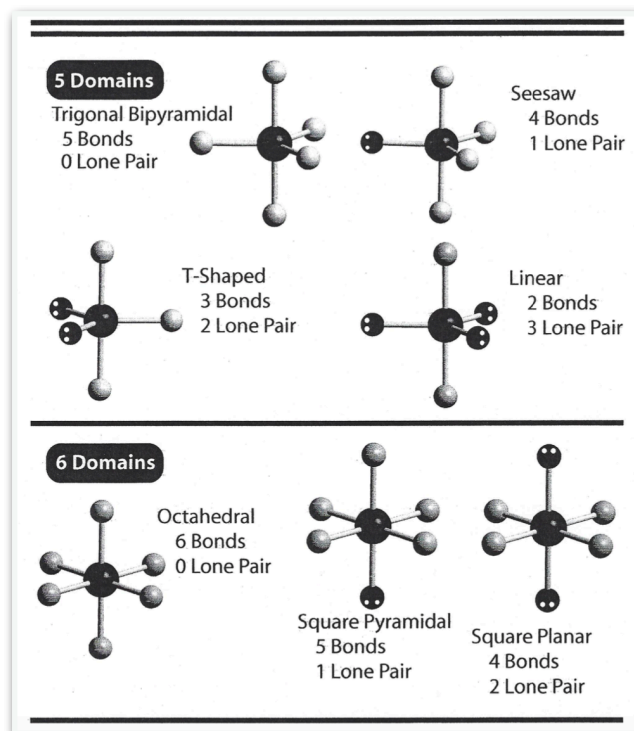
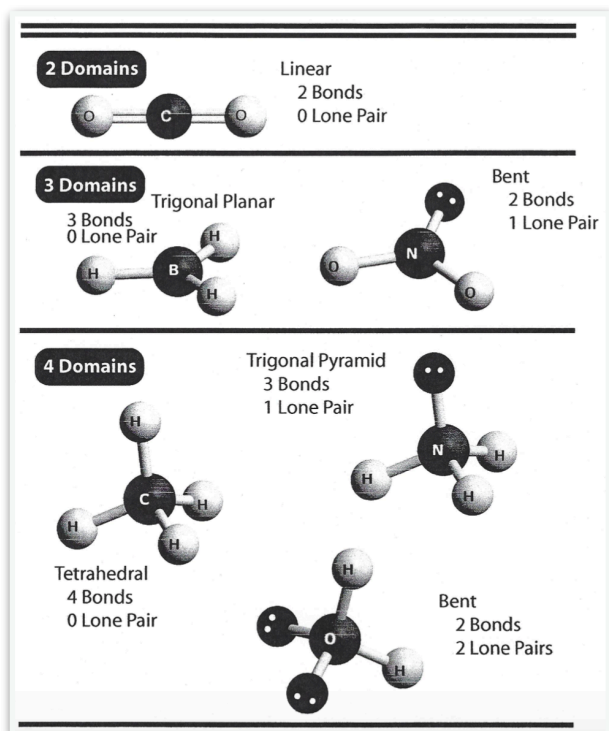


—Every lone pair and bond make up one domain. In the P atom there is one lone pair (one lone pair is two dots) and three bonds, which means there are four domains, one of which is a lone pair. —

- To determine the molecular geometry of a chemical compound you need to count the number of domains it has and how many of those domains are lone pairs. Using that information you can look in a chart to determine the molecular geometry.

Total # of Domains	Bonding Domains	Nonbonding Domains	Molecular Geometry	Bond Angle
2	2	0	Linear	180°
3	3	0	Trigonal Planar	120°
3	2	1	Bent	< 120°
4	4	0	Tetrahedral	109.5°
4	3	1	Trigonal Pyramidal	< 109.5°
4	2	2	Bent	< 109.5°
5	5	0	Trigonal Bipyramidal	120°, 90°
5	4	1	Seesaw	< 120°, < 90°
5	3	2	T-Shaped	< 90°
5	2	3	Linear	180°
6	6	0	Octahedral	90°
6	5	1	Square Pyramidal	< 90°
6	4	2	Square Planar	90°

- Pictures of the shapes of the molecules are shown below:



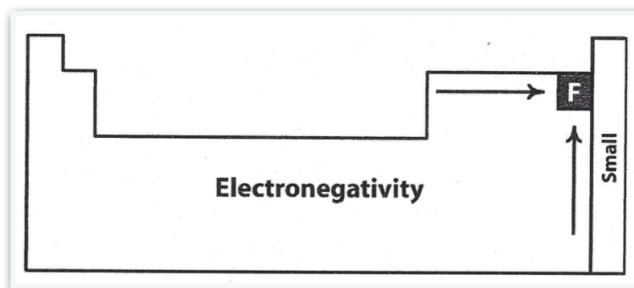
**BEWARE:** If a chemical only has two atoms it will always be linear for example O<sub>2</sub>.

- The molecular geometry of a chemical describes the shapes and bond angles between atoms. An electron domain geometry takes into account the lone pairs that make up the chemical. To determine the electron domain geometry you can use the following chart.

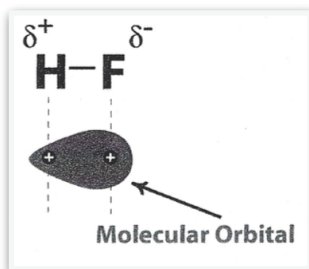
Electron Domain Geometry	Hybrid Orbitals
2 domains (Linear)	$sp$
3 domains (Trigonal planar)	$sp^2$
4 domains (Tetrahedral)	$sp^3$
5 domains (Trigonal bipyramidal)	$sp^3d$
6 domains (Octahedral)	$sp^3d^2$

## Polar vs Non polar

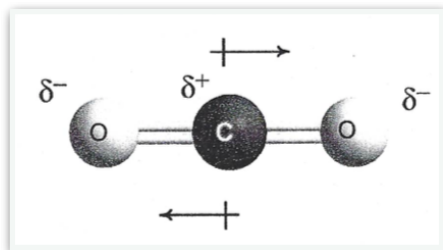
- To determine if a chemical is polar or non polar you need to take into account the 3D shape of the molecular geometry and the direction of the pull of electrons.
- We just went over how to determine the 3D shape of electrons, but not the pull of electrons. To determine the pull of electrons you need to compare the electronegativity of the two atoms. The more electronegative the atom the more electrons will be attracted to it and that atom will have a slight negative charge.



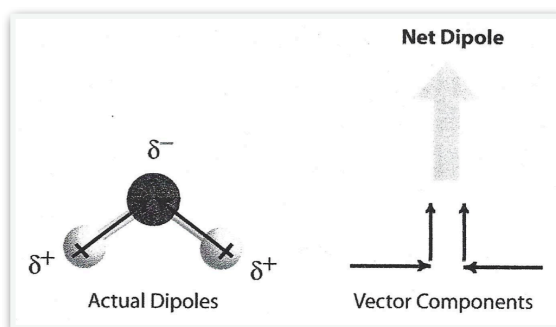
- For example, if we compare the electronegativity of HF, F is more electronegative which means the 2 electrons that are apart of that bond will be pull more towards the F than the H and as a result the F will be slightly negative.



- Because there are two different pulls (one negative and one positive) in HF, we say that HF is polar.
- For chemicals that are not linear we need to take into account the different pulls of electrons in the different directions. For example look at the lewis structure for CO<sub>2</sub>.



- Even though oxygen is more electronegative than carbon the pulls of the different oxygens cancel each other out because the molecule is linear. However, if this molecule was bent they would not cancel out, like in H<sub>2</sub>O.



- The following pictures shows some different combinations of polar and nonpolar molecules.

Nonpolar		Polar	
 5 Identical Domains	5 Domains	 At least 1 Different Equatorial Domain	
		 1 Different Axial Domain	
 6 Identical Domains	6 Domains	 2 Identical Domains at 90° 4 Identical Domains	
		 2 Identical Domains at 180° 4 Identical Domains	

Nonpolar		Polar	
 2 Identical Domains	2 Domains	 2 Different Domains	
 3 Identical Domains	3 Domains	 At Least 1 Different Domain	
 4 Identical Domains	4 Domains	 At Least 1 Different Domain	