Valence Shell Electron-Pair Repulsion - VSEPR

- Method to convert a simple Lewis Formula into a 3-D shape.

- The 3-D structure is predicted by minimizing the electron-pair repulsions between unshared pairs and the e^- on the surface of adjacent atoms and the electron pairs in bonds.

- Molecular shape is based on the 3-D arrangement of atoms joined by bonds.

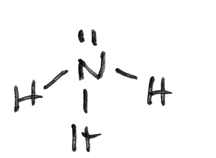
- Electron-pair or electron group arrangement influences the position of the external atoms bonded to the central atom. Again, the shape is defined based on the arrangement of atoms around the central atom.

- There are two types of e^- pairs: bonding e^- and nonbonding e^- pairs.

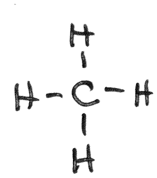
  — = $2e^-$ = bonding pair

  •• = $2e^-$ = unshared pair e^- = nonbonding e^-

- The e^- pair arrangement may not be the same as the molecular shape. Below is an example:



pyramidal



tetrahedral

The NH_3 and CH_4 have the same electronic geometry but different molecular shape. This is because the shape is defined by arrangement of the external atoms not e^- pairs.

However, we can use the e^- pair arrangement to predict molecular shape because the two issues are related and there are repeating trends.

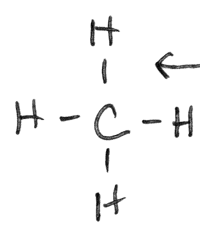
Predicting molecular shape from electronic shape requires two steps:

1) First determine hybridization
2) Use hybridization to find molecular shape.

Hybridization

when two atoms form a covalent bond they do this by mixing or hybridizing their atomic orbitals into molecular orbitals. Atoms do this by mixing s, p, and d orbitals. we call this mixing - hybridization. The hybridization represents the electronic arrangement of e^- pairs around the central atom. A particular hybridization is tied to a specific molecular shape.

To find hybridization for simple molecules assume the mixing is sp^x where s is an s orbital and p is a p orbital and x is the # of p orbitals utilized to form the molecular orbital. This process is easier than it sounds. For example, determine the hybridization of:

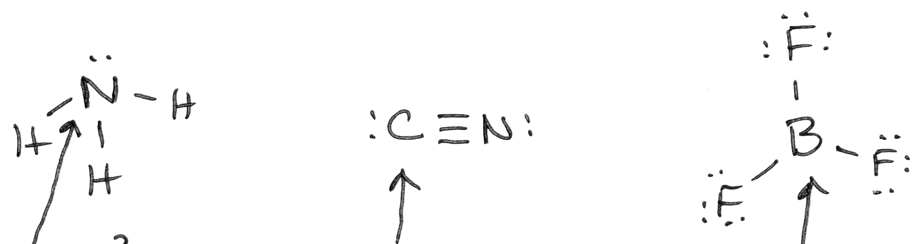


count the total bonding and nonbonding (unshared pairs) pairs and subtract 1.

So sp^x is sp^3

Another example

Determine the hybridization of the central atom.

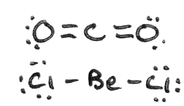
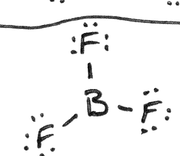
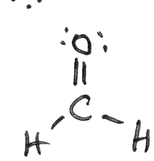


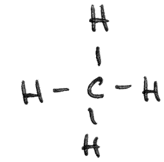
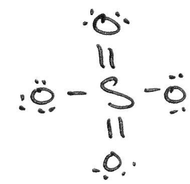
sp^3 $\qquad$ sp $\qquad$ sp^2

In each case the total bonding units were counted and then 1 was subtracted to give the x in sp^x.

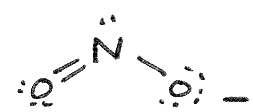
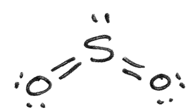
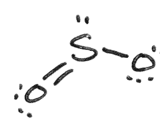
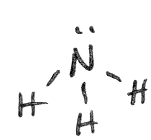
Single bond = 1 bonding unit
double bond = 1 bonding unit
triple bond = 1 bonding unit
•• = 1 bonding unit

Now we will tie hybridization to molecular shape:

Hybridization	Examples	Shape	Bond angles	Drawing
sp	$BeCl_2$, CO_2	linear	180°	
sp^2	BF_3, CH_2O	Trigonal planar	120°	 

Hybridization	Examples	Shape	Bond Angles	Drawing
sp^3	CH_4	tetrahedral	109.5	
	SO_4^{-2}			

Exceptions

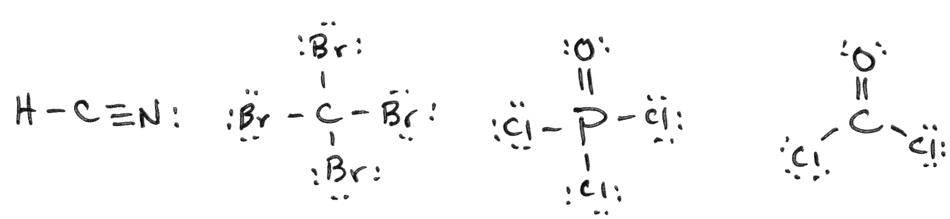
sp^2	NO_2^-	bent	$x < 120°c$	
	SO_2			 
	O_3			
sp^3	H_2O	bent	$x < 109.5$	
sp^3	$\ddot{N}H_3$	pyramidal	$x < 109.5$	

Examples

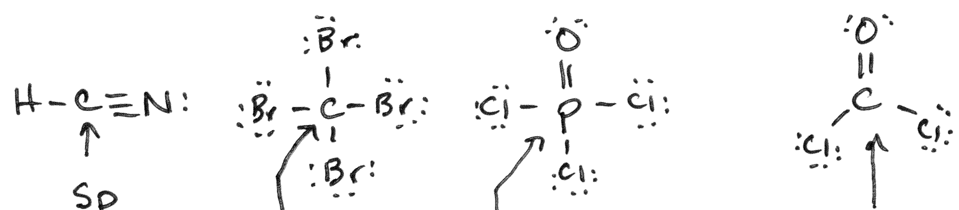
Determine the shape and bond angles of the following molecules:

HCN, CBr_4, $POCl_3$, $COCl_2$

1. First draw <u>best</u> LF:



2. Determine sp^x on central atom:



sp $\quad$ sp^3 $\quad$ sp^3 $\quad$ sp^2

linear $\quad$ tetrahedral $\quad$ Trigonal planar

3. Have memorized chart so