Molecular Shape and VSEPR

Unit One

Lewis Structure

- Atoms want to achieve Noble Gas configuration through bonds

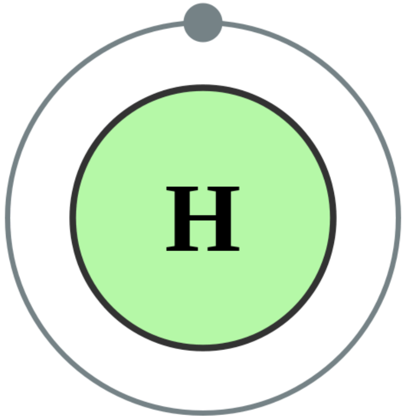
The Octet Rule – atoms tend to have 8 electrons in the valence shell which makes them stable and unreactive

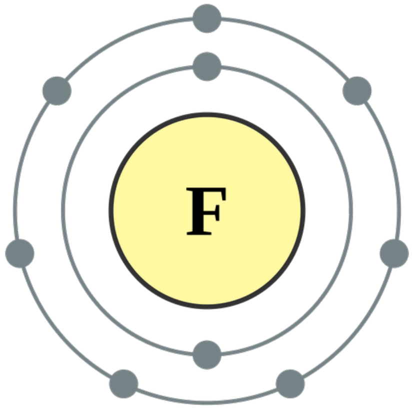
The larger the molecule/polyatomic ion becomes … the more likely there may be an exception to the "Octet Rule"

Lewis Structures for Simple Molecules/Ions

1. The least electronegative atom should be positioned as the "Central Atom"

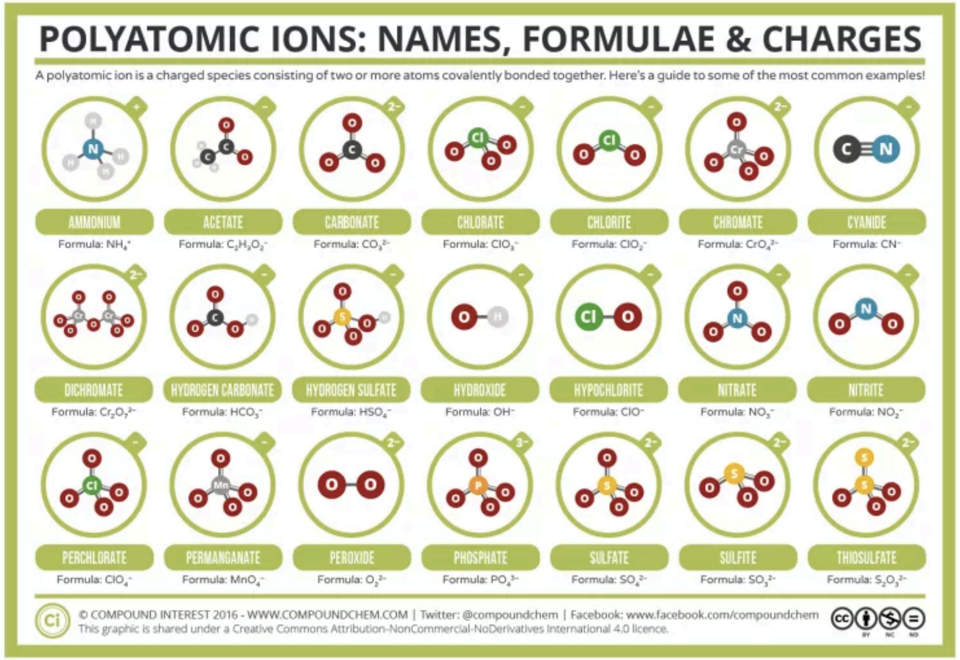
2. Hydrogen or Fluorine at positioned at 'the end' of a structure
    1. They will never be a central atom





Lewis Structures

3. Determine total number of valence electrons
    3. Watch out for charges – especially on polyatomic ions



4. Determine the total number of electrons needed for every atom to achieve noble gas electron configuration

Lewis Structure

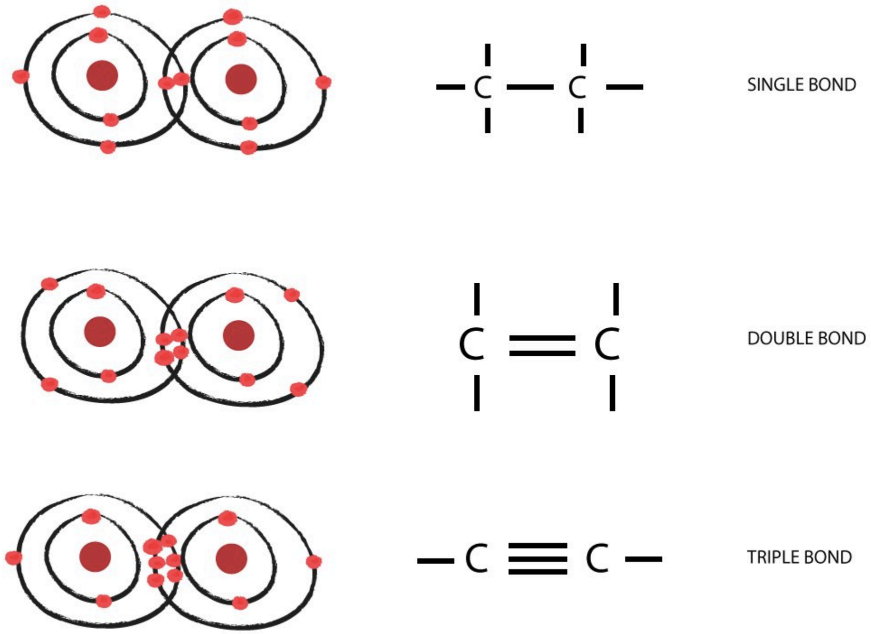
5. Subtract # of valence electrons from # needed to satisfy octet rule

    (how many you have from how many you need)

6. Divide this number by 2 to determine the number of bonds

    Double bonds – count as 2 bonds

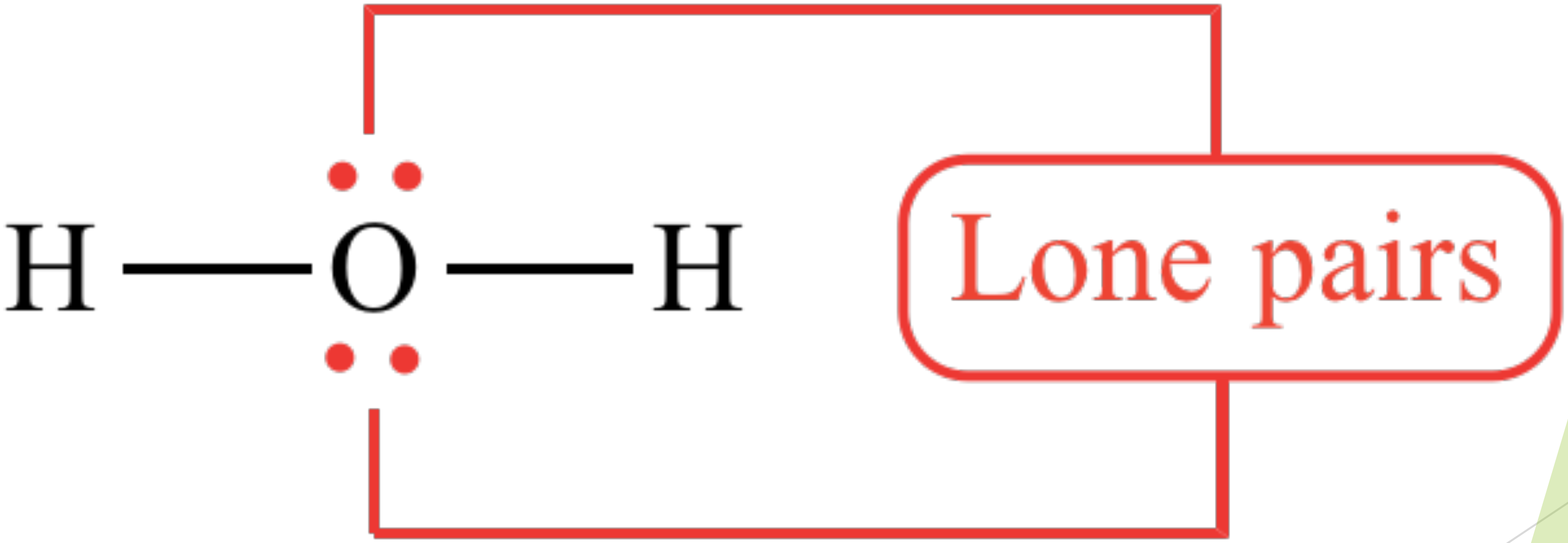
    Triple bonds – count as 3 bonds



Lewis Structure

7. Subtract the number of shared electrons from the number of valence electrons

    Add them as lone pairs to achieve noble gas electron configuration



EXAMPLE

Fromaldehyde (Methanal)

$$CH_2O$$

Following the steps outlined we can determine the molecular formular

Methanal

- Composed of H and C and O
  - We know H has to be placed at the "end" meaning C or O our central atom
  - C has a lower electronegativity than O therefore C is our central atom

H

H

C EN = 2.55

O EN = 3.44

Methanal

- Determine the number of valence electrons

1 C atom * 4 e^-/C atom = 4 electrons

+

1 O atom * 6 e^- /O atom = 6 electrons

+

2 H atoms * 1 e^- / H atom = 2 electrons

12 valence electrons

Methanal

- Electrons needed for full valence shells

C – needs 8

O – needs 8

H – needs 2

= 8 + 8 + (2)2 = 20 electrons

Methanal

- Find the number of shared electrons

Valence Needed – Valence Total
$= 20\ e^- - 12\ e^-$
$= 8\ e^-$

Number of bonds
Shared electrons / 2
$= 8\ e^- / 2$
= 4 bonds

Methanal

- Find the number of non-bonding electrons

Total Valence Electrons – Shared Electrons

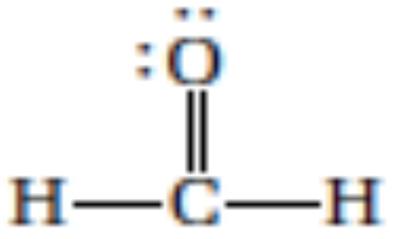
$= 12\ e^- - 8\ e^-$

$= 4\ e^-$

Since electrons are always found in pairs – we know that 4 electrons = 2 non-bonding pairs

Methanal

- We know there are four bonds – but from our initial structure we only have 3



We must add another bond – where?

H can only make one bond, therefore it must be between O and C

You Try!

- NH_3
- CF_4
- CH_4
- AsH_3
- H_2S
- ClNO

Lewis Structure for More Complex Structures

- Co-Ordinate Covalent Bonds
  - Covalent – sharing of electron pairs

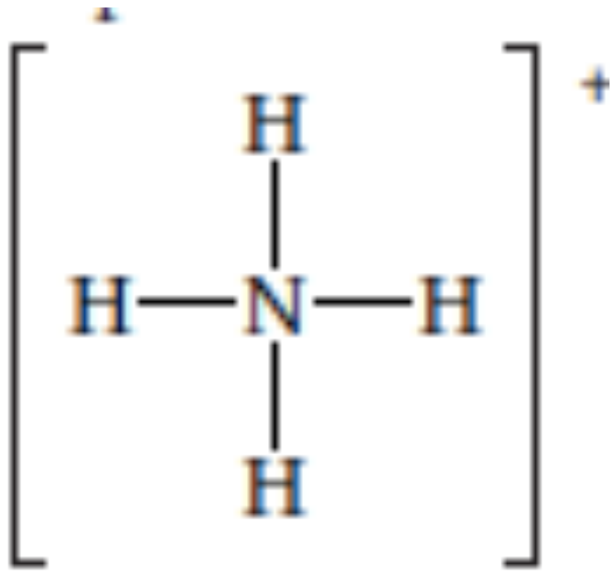
When a filled atomic orbital overlaps with an empty atomic orbital

Ex. NH_4^+

Ammonium

- NH_4^+ - N is central atom, H is surrounding
- Valence Electrons
  - 1 N ($5e^-$) + 4H ($1e^-$) – $1e^-$ = 8 electrons
- Noble Gas Electrons
  - 1 N ($8e^-$) + 4H ($2e^-$) = 16 electrons
- Number of Shared / Bonds
  - 16 electrons – 8 electrons = 8
  - 8 electrons / 2 electrons/bond = 4 bonds
- Number of non-bonding (unpaired) electrons
  - 8 valence electrons – 8 shared electrons = 0 lone pairs

Ammonium



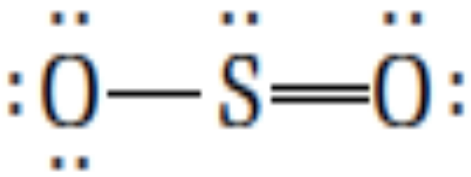
Possible structure

Try It!

- BrO^-
- H_2O_2

Resonance Structures

SO_2

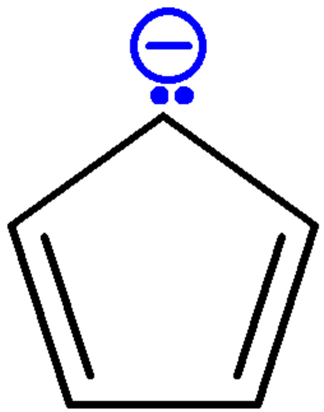


to satisfy the Octet Rule

Give the same relative position of atoms, with different places for bonding and lone pairs

Resonance Structures

- Required by Molecules and Ions
- Not “real” – but a weighted average between multiple structures

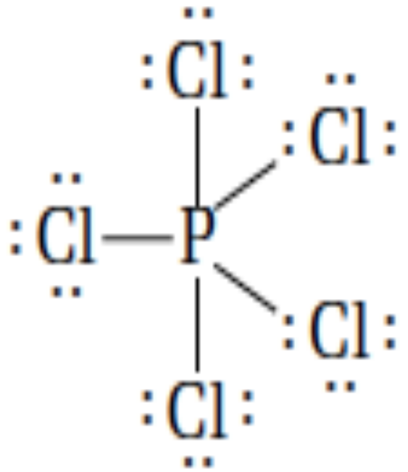


Try These!

- CO_3^{2-}
- NO^+
- ClO_3^-
- SO_3^{2-}

Expanded Valence Level

- An exception to the octet rule
- Allows central atoms to maintain more than 8 electrons in the valence energy
- Arose from experiments and measurements of bond energies



Phosphorus Pentachloride

Try These!

- SF_6
- BrF_5
- XeF_4
- PF_5

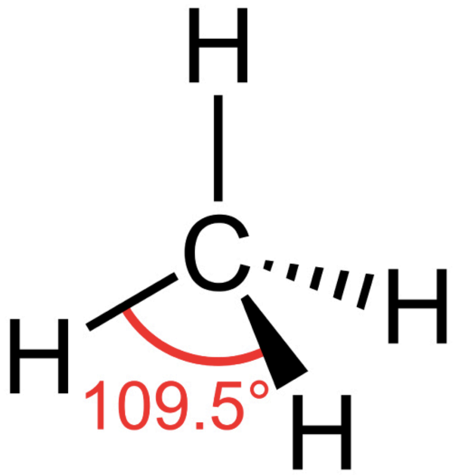
VSEPR

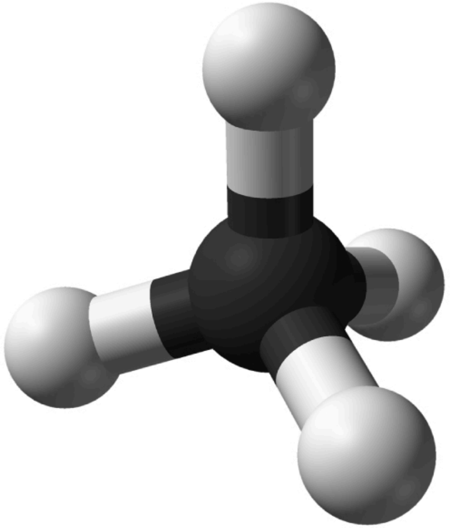
- Valence Shell Electron Pair Repulsion Theory
  - Ronald Gillespie and Ronald Nyholm (1957)

Bonding and lone pairs in a valence levels of an atom repel one another. These electron pairs are “localized” in orbitals and will try to be as far apart from one another as they can in order to minimize energy

Indicating 3D Shapes

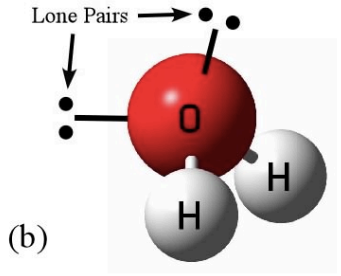
Names of types of chemical bonds used to draw 3D molecular structures:		Orientations of chemical bonds indicated by these styles:
"normal" bond	———	bond lies in the plane of the paper (*or screen, when viewed electronically*)
dashed bond	- - - - - - -	bond extends backwards, away from the viewer, so effectively "into" the paper (*or screen*)
wedged bond	◀	bond protrudes forwards, towards the viewer, so effectively "out of" the paper (*or screen*)



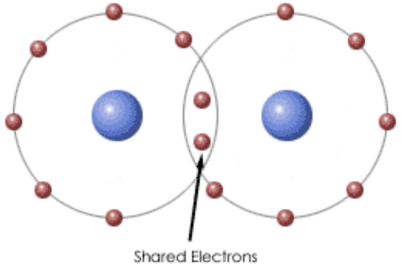


Optimized Shape

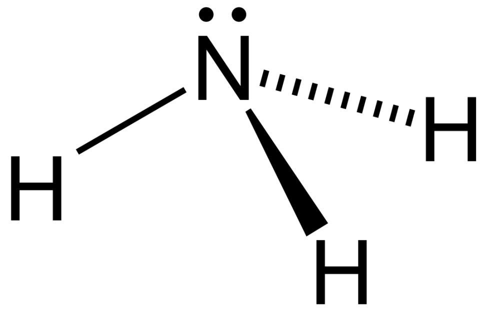
Lone Pairs (LP-LP) will have the greatest repulsion and spread apart the most



Bonding Pairs (BP-BP) are localized between two nuclei and restricted in their ability to spread out



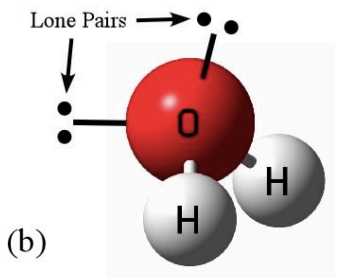
Lone-Bonding Pairs (LP-BP) have a 'hybrid' repulsion that is intermediate between the other two

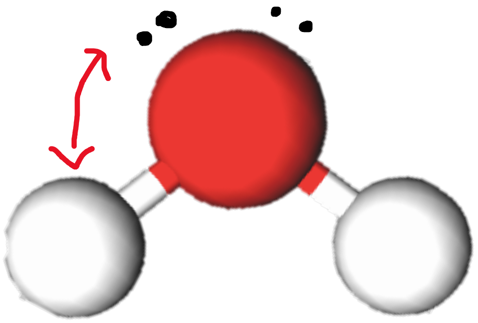


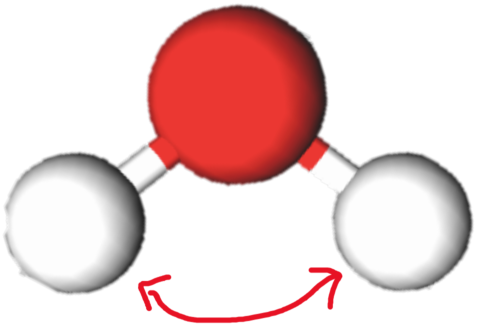
Optimized Shape

$$LP\!-\!LP > LP\!-\!BP > BP\!-\!BP.$$

Greatest repulsion

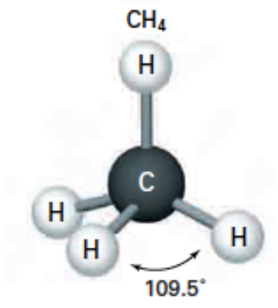




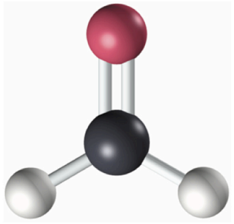


5 Basic Geometrical Arrangements

Carbon with 4 single bonds: tetrahedral



Carbon with a double bond: trigonal planar



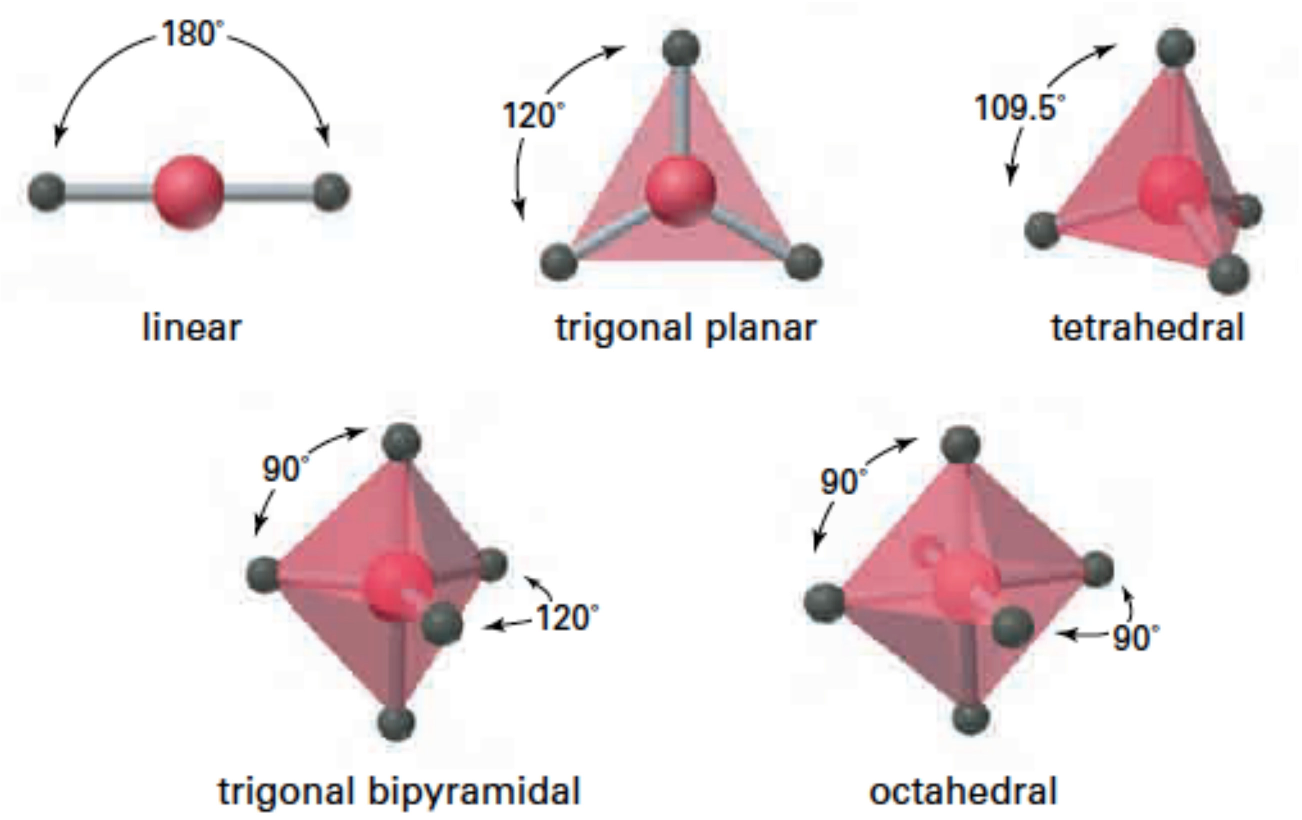
Carbon with a triple bond: linear

Why these shapes?

Because of lone pair and bonding pair repulsions!

If all electron groups are bonded – the shape is one of the five basic
If there are one or more lone pairs – there are variations that occur

5 Basic Geometric Shapes



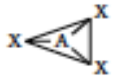
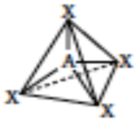
Based off total number of electron groups

VSEPR Theory (Molecular Geometry)

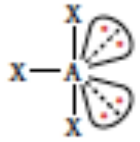
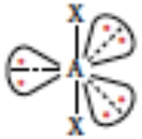
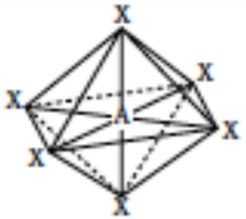
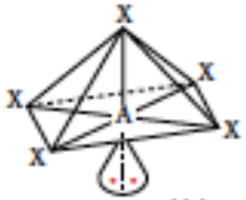
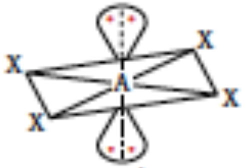
Number of Electron Dense Areas	Electron-Pair Geometry	Molecular Geometry				
		No Lone Pairs	1 lone Pair	2 lone Pairs	3 lone Pairs	4 lone Pairs
2	Linear	Linear				
3	Trigonal planar	Trigonal planar	Bent			
4	Tetrahedral	Tetrahedral	Trigonal pyramidal	Bent		
5	Trigonal bipyramidal	Trigonal bipyramidal	Sawhorse	T-shaped	Linear	
6	Octahedral	Octahedral	Square pyramidal	Square planar	T-shaped	Linear

Specifies types of electron groups

VSEPR

Number of electron groups	Geometric arrangement of electron groups	Type of electron pairs	VSEPR notation	Name of Molecular shape	Example
2	linear	2 BP	AX_2	X—A—X linear	BeF_2
3	trigonal planar	3 BP	AX_3	 trigonal planar	BF_3
3	trigonal planar	2 BP, 1 LP	AX_2E	 angular	$SnCl_2$
4	tetrahedral	4 BP	AX_4	 tetrahedral	CF_4
4	tetrahedral	3 BP, 1LP	AX_3E	 trigonal pyramidal	PCl_3
4	tetrahedral	2 BP, 2LP	AX_2E_2	 angular	H_2S
5	trigonal bipyramidal	5 BP	AX_5	 trigonal bipyramidal	$SbCl_5$
5	trigonal bipyramidal	4 BP, 1LP	AX_4E	 seesaw	$TeCl_4$

VSEPR

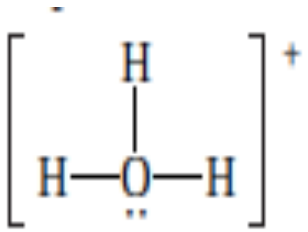
5	trigonal bipyramidal	3 BP, 2LP	AX_3E_2	 T-shaped	BrF_3
5	trigonal bipyramidal	2 BP, 3LP	AX_2E_3	 linear	XeF_2
6	octahedral	6 BP	AX_6	 octahedral	SF_6
6	octahedral	5 BP, 1LP	AX_5E	 square pyramidal	BrF_5
6	octahedral	4 BP, 2LP	AX_4E_2	 square planar	XeF_4

Predicting Molecular Shape

- Draw a preliminary Lewis Structure based on formula
- Determine total number of electron groups around central atom
  - Double/Triple bonds count as one electron group
- Determine which geometric arrangement accommodates the total number of electron groups
- Determine molecular shape

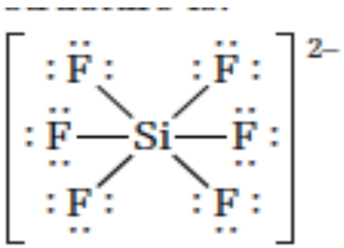
H_3O^+

Determine Molecular Shape of H_3O^+

- Possible Structure: 
- Bonding/Lone Pairs: On oxygen – 3 bonding pairs, 1 lone pair
  4 groups total
- Geometrical Shape: Of the five basic shape – 4 groups is Tetrahedral
- Molecular Shape: With 3 BP and 1 LP the molecular shape is Trigonal Pyramidal

SiF_6^{2-}

Determine Molecular Shape of SiF_6^{2-}

- Lewis Structure:  Silicon has an expanded valence shell
- Bonding/Lone Pairs: Central atom has 6 BP and 0 LP
  6 groups total
- Geometrical Shape: Of the five basic shapes 6 groups:
  Octahedral
- Molecular Shape: For 6 BP the Molecular Shape is:
  Octahedral

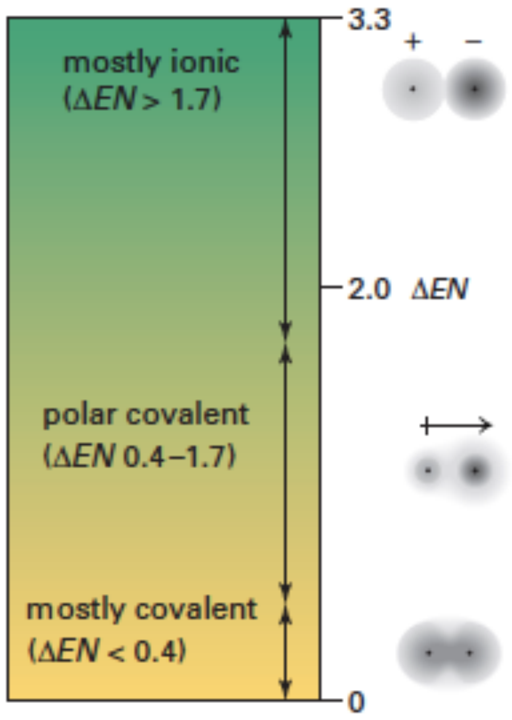
Try These!

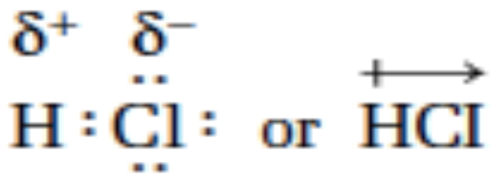
Determine the geometric and molecular shape for the following:

$BrCl_4^-$	CH_2F_2
HCN	$AsCL_5$
SO_2	NH_4^+
SO_3	BF_4^-
SO_4^{2-}	

Shape and Polarity

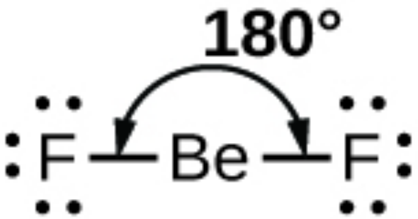
Shape and Polarity are directly related

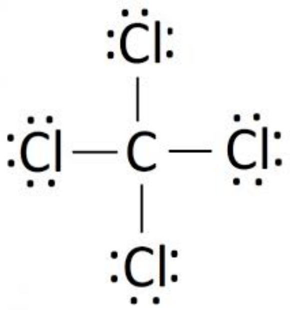


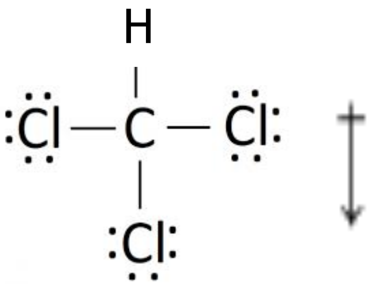


Dipole

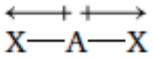
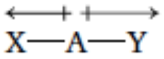
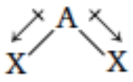
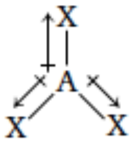
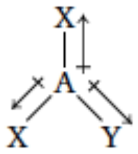
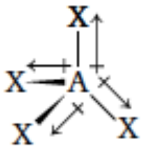
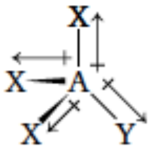
- In diatomic molecules bond polarity applies to the overall molecule
- Polyatomic molecules relies on all the bonds and angles and where they “come together”







Shape and Polarity

Molecular shape	Bond polarity	Molecular polarity
linear		non-polar
linear		polar
bent		polar
trigonal planar		non-polar
trigonal planar		polar
tetrahedral		non-polar
tetrahedral		polar

Try These!

Use VSEPR Theory to predict the shape of the following molecules.

Determine whether the molecule is polar or not.

CH_3F CH_2O GAI_3