Covalent Bonding
Nomenclature
Lewis structure
Resonance
VSEPR theory
Molecular Polarity

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Binary Covalent Compounds: Two Nonmetals (such as CO_2)

1. Name first element in formula first
   - ✓ use the full name of the element
2. Name the second element in the formula with an **-ide**
   - ✓ as if it were an anion, *however, remember these compounds do not contain ions*!
3. Use a prefix in front of each name to indicate the number of atoms
   a) Never use the prefix ***mono-*** on the first element

Subscript - Prefixes

- 1 = mono-;
  - ✓ not used on first nonmetal
- 2 = di-
- 3 = tri-
- 4 = tetra-
- 5 = penta-
- 6 = hexa-
- 7 = hepta-
- 8 = octa-
- drop last “a” if name begins with vowel

Exceptions when Naming Covalent Compounds

of course, water ☺

Other common exceptions:

- **NH_3: ammonia** (as in *Windex*)
- H_2S: hydrogen sulfide
- HCl: hydrogen chloride (same for HX, where X = halogen)
- **CH_4: methane** (as in natural gas)
- H_2O_2: hydrogen peroxide

Example – Naming Covalent Molecular
BF_3

1. Is it one of the common exceptions?
2. Ionic or Covalent compound?
3. Covalent: using prefixes for noncommon exceptions.

Practice:

Naming Covalent Compounds

- CO
- ClO_2
- SO_3
- P_2O_5
- N_2O_4
- IF_7
- SF_6

Key to Naming Molecular Compounds

- CO — *carbon monoxide*
- ClO_2 — *chlorine dioxide*
- SO_3 — *sulfur trioxide*
- P_2O_5 — *diphosphorus pentoxide*
- N_2O_4 — *dinitrogen tetroxide*
- IF_7 — *iodine heptoxide*
- SF_6 — *sulfur hexafluoride*

Lewis Bonding Theory

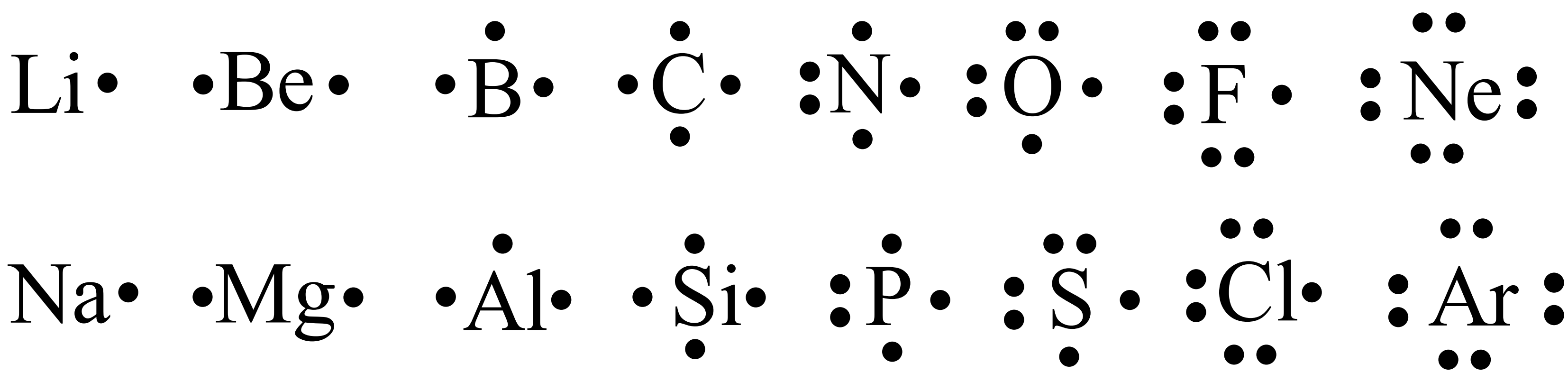
- Atoms bond because bonding results in a more stable Electron Configuration

- by either <u>transferring</u> or <u>sharing</u> electrons so that all atoms obtain an Outer Shell with **8** electrons
  - → **Octet Rule**
    - ✓Some exceptions: H, He, Li, Be.
    - ✓How to remember? Everyone wants to have an electron configuration like a Noble Gas

Lewis Symbols of Atoms

also <u>Electron Dot Symbols</u>

- Symbol of element : Nucleus and Inner electrons
- Dots: around the Symbol as Valence electrons
  - ✓ put one electron on each side first, then pair
  - ✓ elements in the same group have the same number of valence electrons → same Lewis dot symbols



Lewis Formulas of Molecules

Also Lewis Structure:

- pattern of <u>Valence electron distribution</u>
- understand the bonding in many compounds
- predict <u>Shapes of molecules</u>
- predict <u>Properties of molecules</u> and how they will interact together

Covalent Bonds

Within molecule:

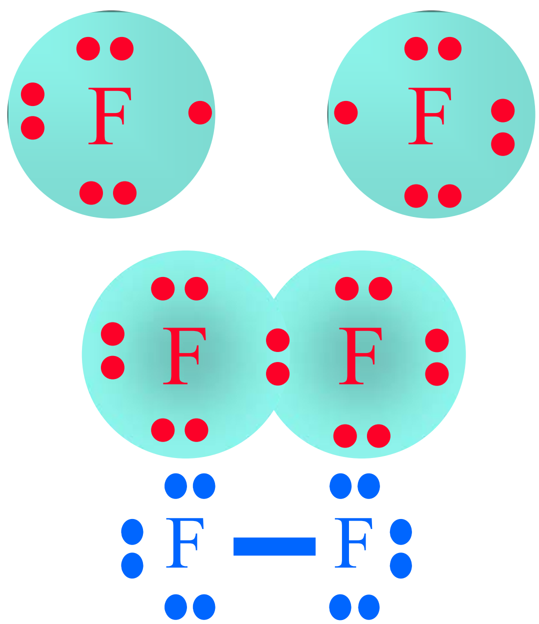
- Often between two Nonmetals
- typical of molecular species: atoms bonded together to form molecules
  - ✓ strong attraction
- **sharing pairs of electrons** to attain **Octets**

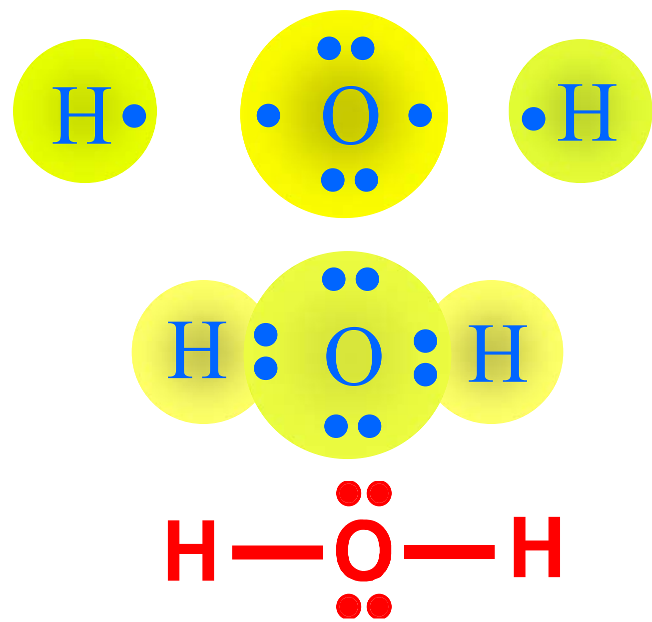
Between molecules: molecules generally weakly attracted to each other

- ✓ observed physical properties of molecular substance due to these attractions

Single Covalent Bonds

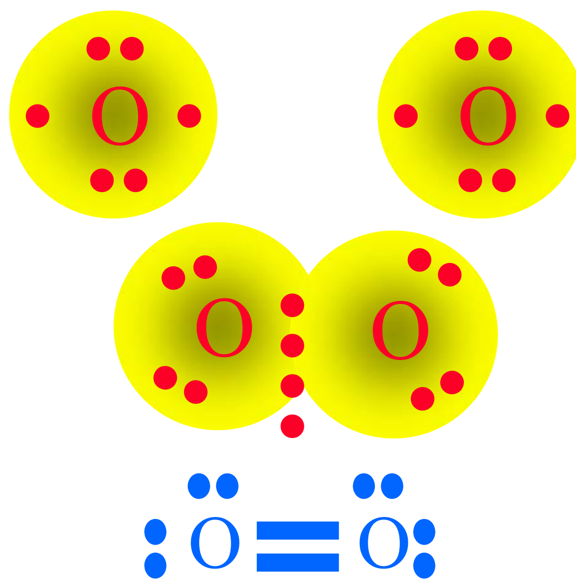
- two atoms share ONE pair of electrons
  - ✓ 2 electrons
- one atom may have more than one single bond





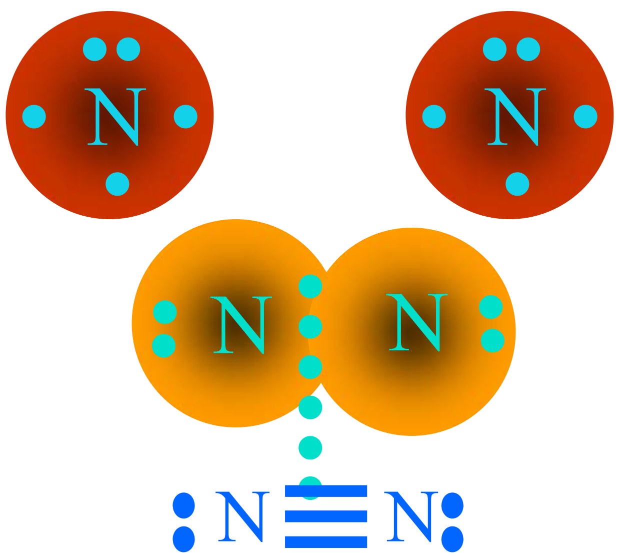
Double Covalent Bond

- two atoms sharing TWO pairs of electrons
  - ✓4 electrons
- shorter and stronger than single bond: O_2

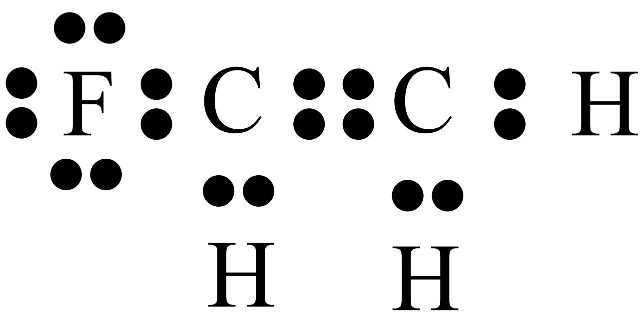


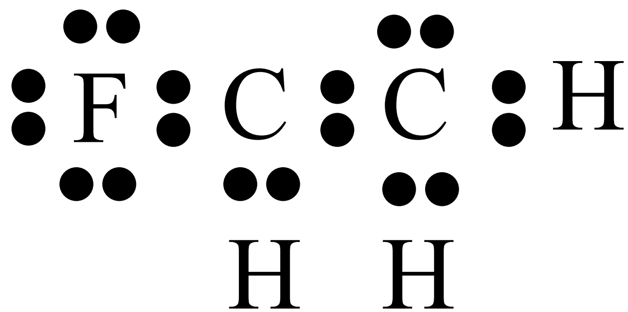
Triple Covalent Bond

- two atoms sharing 3 pairs of electrons: N_2
  - ✓6 electrons
- shorter and stronger than single or double bond



Practice: Which one(s) violate the Octet Rule?

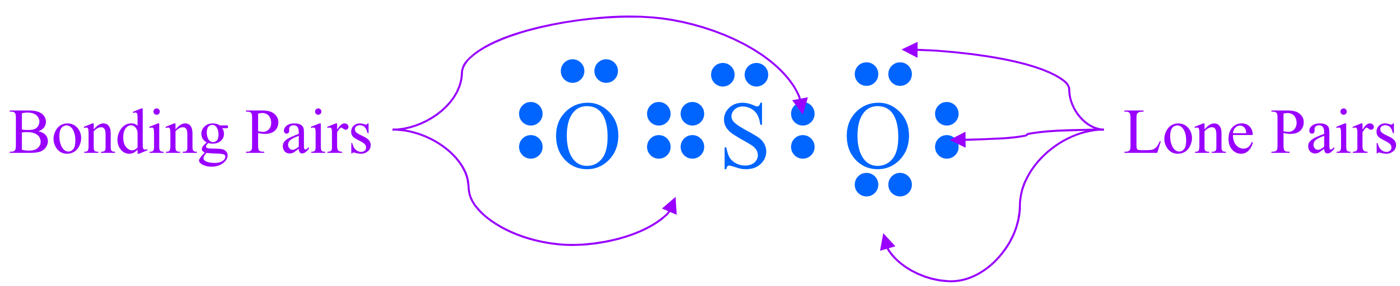




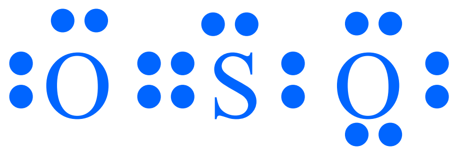
Bonding & Lone Pair Electrons

- **Bonding pairs** : Electrons shared by atoms
- **Lone pairs :** Electrons that are not shared by atoms but belong to a particular atom (also known as **nonbonding pairs)**

Example: SO_2



Practice: Count Bonding Pairs and Lone Pairs



- How many Lone pair(s) on Sulfur?
- How many bonding pairs on Oxygen to the left?

Polyatomic Ions: $\mathbf{NH_4^+}$ …$\mathbf{NO_3^-}$

- Polyatomic ions are attracted to opposite ions by ionic bonds
  - ✓Form crystal lattices

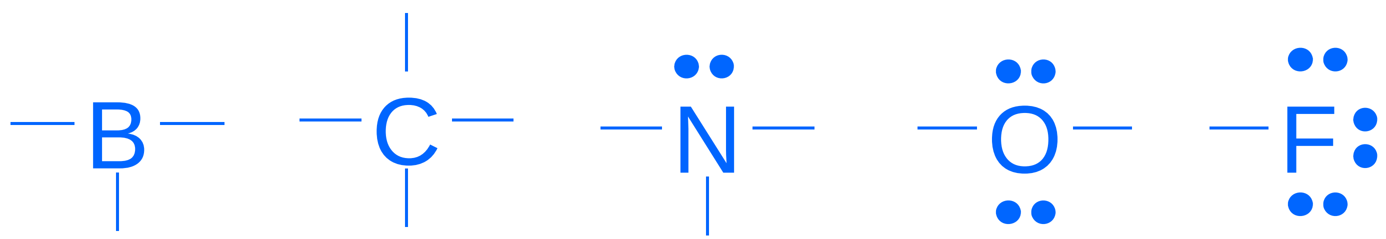
- Atoms within the polyatomic ion are held together by ***covalent bonds***

Example:

- Covalent N-H bonds within $\mathbf{NH_4^+}$

Lewis Structures: common bonding patterns

- ✓**C** = 4 bonds & *0 lone pairs*
  - ➢4 bonds = 4 single, or 2 double, or single + triple, or 2 single + double
- ✓**N** = 3 bonds & *1 lone pair*
- ✓**O** = 2 bonds & *2 lone pairs*
- ✓**H** and Halogen (**F, Cl, Br**) = 1 bond,
- ✓**Be** = 2 bonds & *0 lone pairs,*
- ✓**B** = 3 bonds & *0 lone pairs* (Not Octet in B!)



HONC Rule for most neutral molecules to help identify central atom

- The numbers of covalent bonds formed on

1	2	3	4
H	O	N	C

More:

F	S?	P?	Si
Cl?	Se?	As?	
Br?			

Lewis Structures for Covalent Molecules

1) Calculate the total number of Valence electrons available for bonding
   - ✓ use group number of periodic table

2) Arrange the atoms and link with single bonds

the more bond an atom can form, the more center it will be placed;

the fewer an element in a formula, the more center it will be placed.

Lewis Structures for Covalent Molecules

3) Attach atoms with pairs of electrons
   - ✓ Start with Terminal atoms to Octet
   - ✓ H only wants 2 electrons
   - ✓ then attach to Central atoms

4) Share electrons (to make multiple bonds) to complete the <u>Octets</u> of all the atoms

Practice: Drawing Lewis Structures
Step by step!

1) *Count all valence electrons*
2) *Lay out electrons and link with single bonds (HONC)*
3) *Attach atoms with pairs of electrons to complete OCTET, starting with terminal atoms*
4) *Complete OCTET for central atoms, building multiple bonds if necessary (except for H)*

CO_2

Practice: Drawing Lewis Structures
Step by step!

- **nitrogen trifluoride**
- **CH_2Cl_2**
- **CH_2S**
- **carbon monoxide**
- **sulfur trioxide**

1) *Count all valence electrons*
2) *Lay out electrons and link with single bonds (HONC)*
3) *Attach atoms with pairs of electrons to complete OCTET, starting with terminal atoms*
4) *Complete OCTET for central atoms, building multiple bonds if necessary (except for H)*

Lewis Structures for Polyatomic Ions

Same procedure, except the difference in counting the Valence electrons:

- Polyatomic Cations: take away electron from the total for each positive charge

NH_4^+ #Valence electrons = $5 + 4 \times 1 - 1 = 8$

- Polyatomic Anions: add electron to the total for each negative charge

SO_3^{2-} #Valence electrons = $6 + 3 \times 6 + 2 = 26$

Resonance

- **Sometimes two or more Lewis structures are possible for a given arrangement of atoms.**
- For example, the bicarbonate ion, HCO_3^-

Practice: Write Lewis Structures for Polyatomic Ions

- Cyanide ion
- Chlorite ion
- Sulfite ion
- Carbonate ion
- Phosphate ion
- Ammonium ion
- Nitrite ion

1) ***Important!*** *Count all valence electrons, charge matters.*
2) *Lay out atoms and link with single bonds (HONC)*
3) *Attach atoms with pairs of electrons to complete OCTET, starting with terminal atoms*
4) *Complete OCTET for central atoms, building multiple bonds if necessary (except for H)*

Exceptions to the Octet Rule

- **H & Li**, lose one electron to form cation
  - ✓ Li now has electron configuration like He
  - ✓ H can also share or gain one electron to have configuration like He
- **Be** : shares 2 electrons to form 2 single bonds
- **B** : shares 3 electrons to form 3 single bonds
- expanded octets for elements in Period 3 or below
  - ✓ using empty valence *d* orbitals
- some molecules have odd numbers of electrons
  - ✓ NO

Molecular Geometry: *Shape of Molecule*

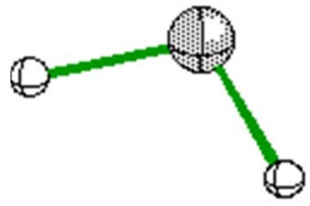
- Molecules are 3-dimensional objects
- Shape of a molecule like Geometric figures

Molecular Geometry indicates

- Positions of the Surrounding atoms with the Central atom in the center of the figure.

Linear, Trigonal, Tetrahedral, Pentagonal, etc.

- **Bond Angles :** angles between adjacent bonds.



in water molecule ∠H-O-H = 105°

Valence Shell Electron Pair Repulsion (VSEPR) theory

- Electron pairs, either bonding or nonbonding, have repulsion against each other and stay apart as much as possible

- Multiple bonds (bonding pairs) occupy one area between two atoms and be treated as ONE electron group

Molecular Geometry depends on
#Electron Groups on Central Atom

- Each Bond counts as 1 Electron group
  - ✓ Single bond
  - ✓ *Double or Triple also as ONE electron group*

Lone Pair "**:**"

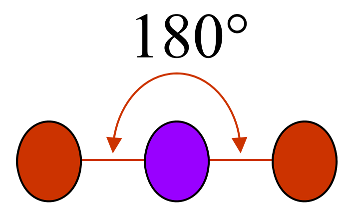
- counts as 1 Electron group
  - ✓ lone pairs "occupy space" around the central atom
- take up slightly more space than bonding pairs
  - ✓ Effects bond angles

Practice: How many Electron Groups on Central Atom

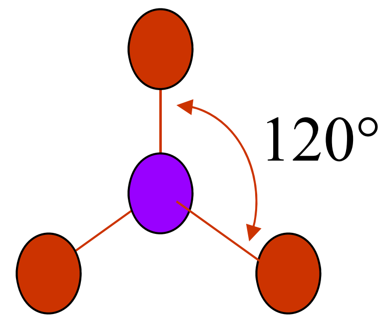
- sulfur trioxide
- sulfite ion
- carbon dioxide
- water
- ammonium ion
- ammonia

Some Geometric Figures

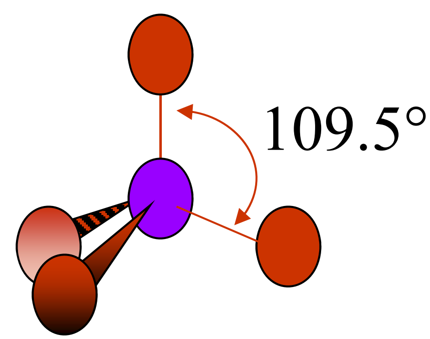
- **Linear** **(e.g, CO_2 or O=C=O)**
  - ✓ 2 atoms on opposite sides of Central atom
  - ✓ Bond angle = 180°



- **Bent** **(e.g, H_2O):** Bond angle < 180°
- **Trigonal Planar** **(e.g, NO_3^-)**
  - ✓ 3 atoms form a <u>Triangle</u> around the Central atom
  - ✓ Planar (all atoms on the same plane)
  - ✓ Bond angles = 120°



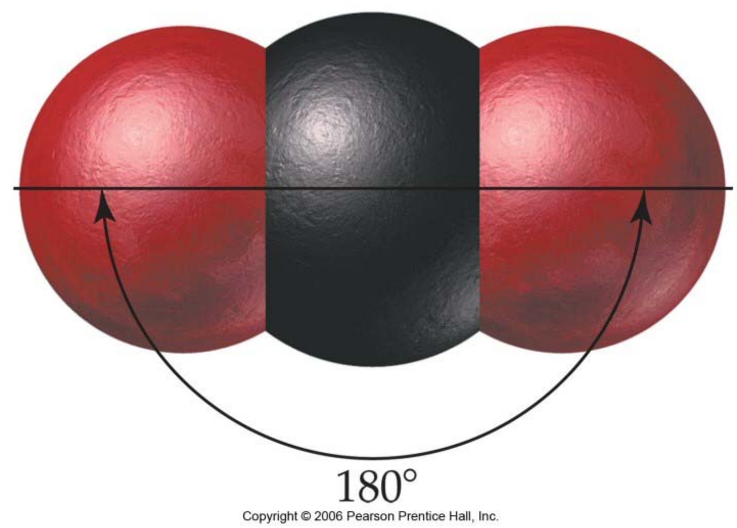
- **Tetrahedral** **(e.g, CH_4)**
  - ✓ 4 atoms form a <u>Tetrahedron</u> around the Central atom
  - ✓ bond angles = 109.5°



Linear Shapes (3 atoms)

- ✓ 2 Electron groups around the **CENTRAL** atom, both Bonding
  - ➢ Or two atom molecule as trivial case
- ✓ Bond Angle = 180°

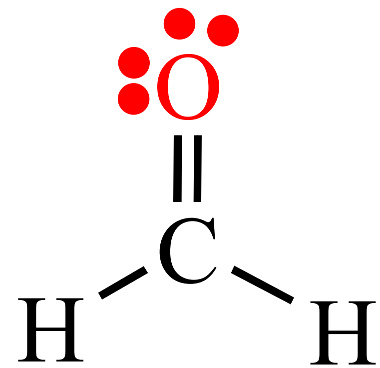
$:\ddot{O} = C = \ddot{O}:$

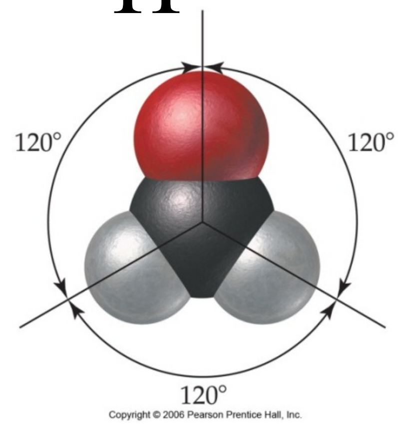


Trigonal Shapes

✓3 Electron groups around the CENTRAL atom

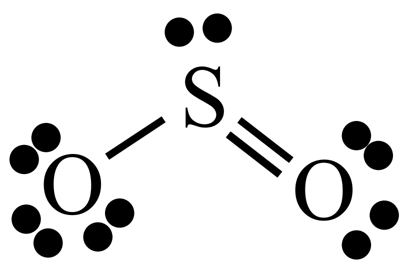
✓bond angles = 120°





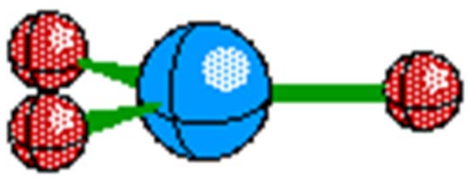
✓All Bonding = **Trigonal planar** **(BF_3 H_2CO, SO_3)**

✓2 Bonding + 1 Lone Pair = **Bent** **(SO_2)**



3D Animation:

Three Electron Groups on Central Atom (bond angle ≈ __________)

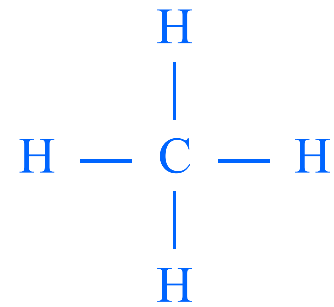


Three terminal atoms
(no lone pair electrons)

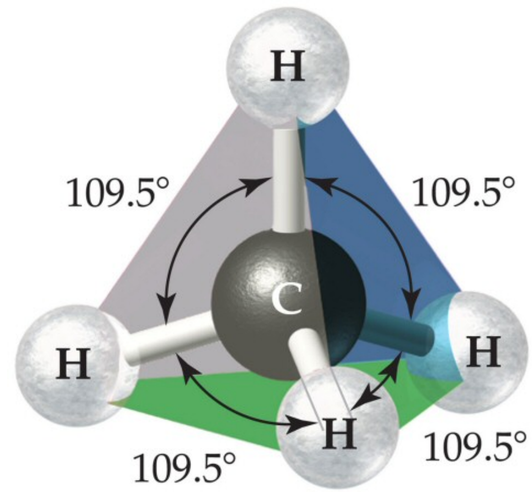
Two terminal atoms
(ONE lone pair electrons)

Tetrahedral Shapes (≥2 atoms)

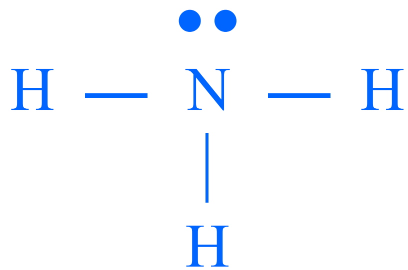
- ✓4 <u>Electron groups</u> around the central atom
- ✓bond angles = 109.5°

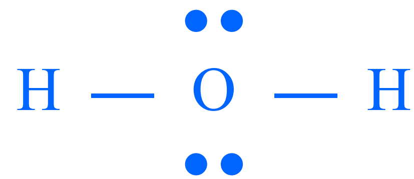


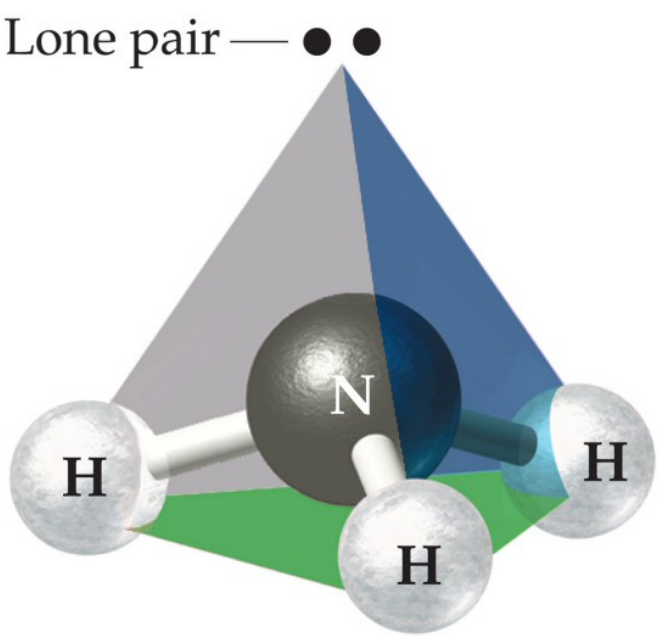
- ✓All Bonding = **Tetrahedral (CH_4, NH_4^+)**
- ✓3 Bonding + 1 Lone Pair Electrons (**LPE**) = **Trigonal pyramid (NH_3)**
- ✓2 Bonding + 2 **LPE** = **Bent (H_2O)**

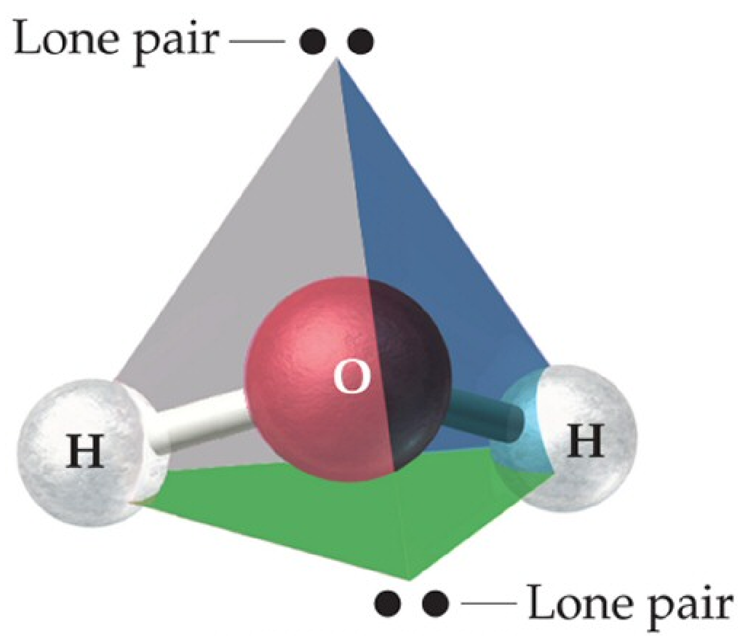


Tetrahedral Derivatives





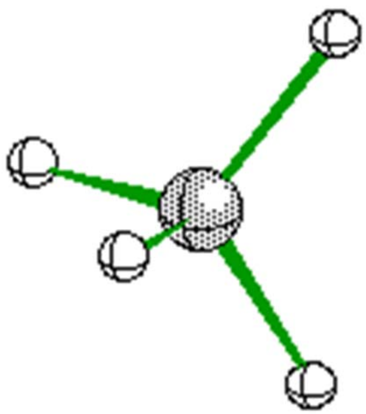




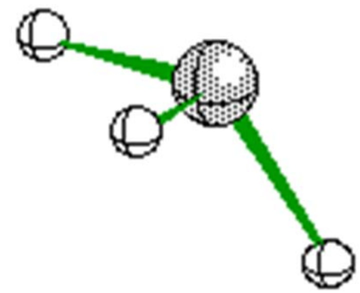
3D Animation:

Four Electron Groups on Central Atom

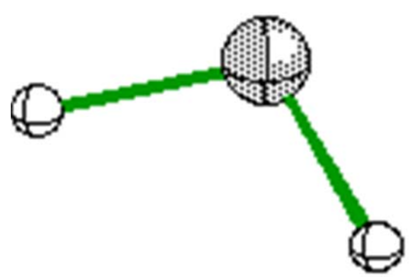
(bond angle ≈ __________)



Four Terminal Atoms
(**Tetrahedral**; no LPE)



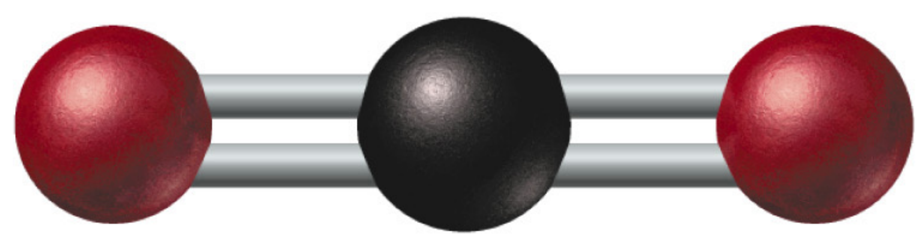
Three Terminal Atoms
(**Trigonal pyramidal**; One LPE)



Two Terminal Atoms
(**Bent**; Two LPE)

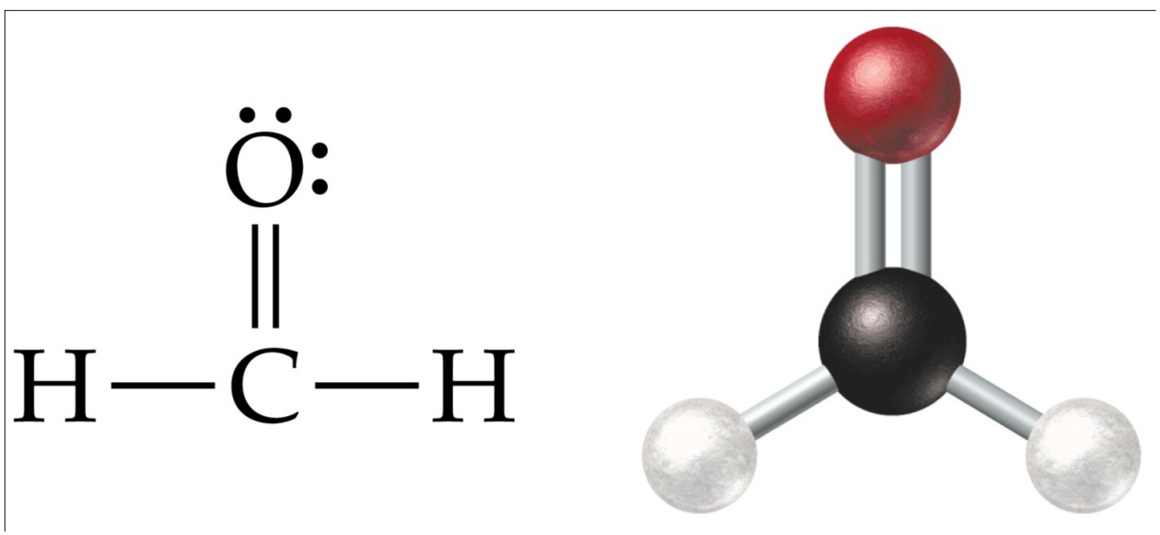
Molecular Geometry: Linear

- Electron Groups Around Central Atom = 2
- Bonding Groups = 2
- Lone Pairs = 0
- Electron Geometry = Linear
- Angle between Electron Groups = 180°



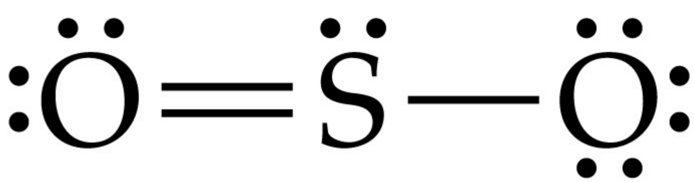
Molecular Geometry: Trigonal Planar

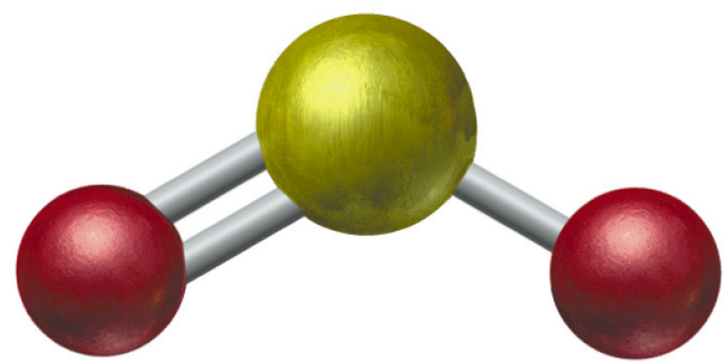
- Electron Groups Around Central Atom = 3
- Bonding Groups = 3
- Lone Pairs = 0
- Electron Geometry = Trigonal Planar
- Angle between Electron Groups = 120°



Molecular Geometry: Trigonal Bent

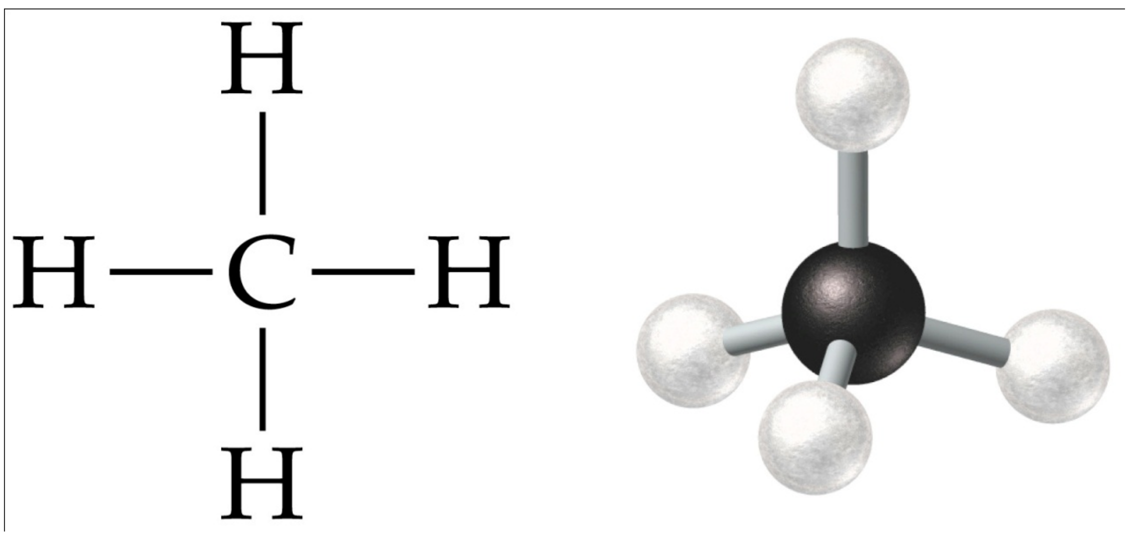
- Electron Groups Around Central Atom = 3
- Bonding Groups = 2
- Lone Pairs = 1
- Electron Geometry = Trigonal Planar
- Angle between Electron Groups = 120°





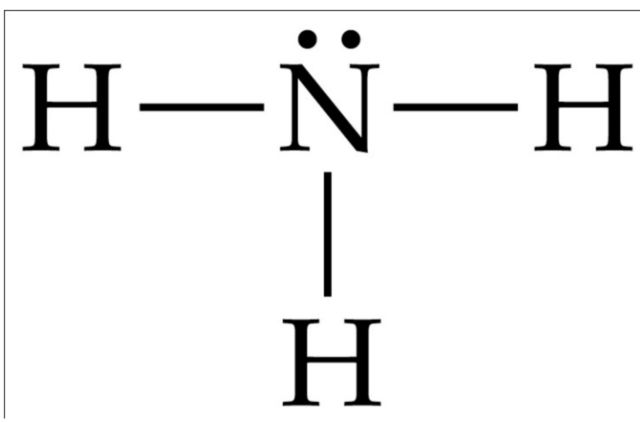
Molecular Geometry: Tetrahedral

- Electron Groups Around Central Atom = 4
- Bonding Groups = 4
- Lone Pairs = 0
- Electron Geometry = Tetrahedral
- Angle between Electron Groups = 109.5°



Molecular Geometry: Trigonal Pyramid

- Electron Groups Around Central Atom = 4
- Bonding Groups = 3
- Lone Pairs = 1
- Electron Geometry = Tetrahedral
- Angle between Electron Groups = 109.5°



Molecular Geometry: Tetrahedral Bent

- Electron Groups Around Central Atom = 4
- Bonding Groups = 2
- Lone Pairs = 2
- Electron Geometry = Tetrahedral
- Angle between Electron Groups = 109.5°

Practice: Determine the Shape and Bond Angle for the following species

- sulfur trioxide
- perchlorate ion
- sulfite ion
- nitrite ion
- carbon disulfide
- ammonium ion
- hydrogen cyanide
- carbonate ion

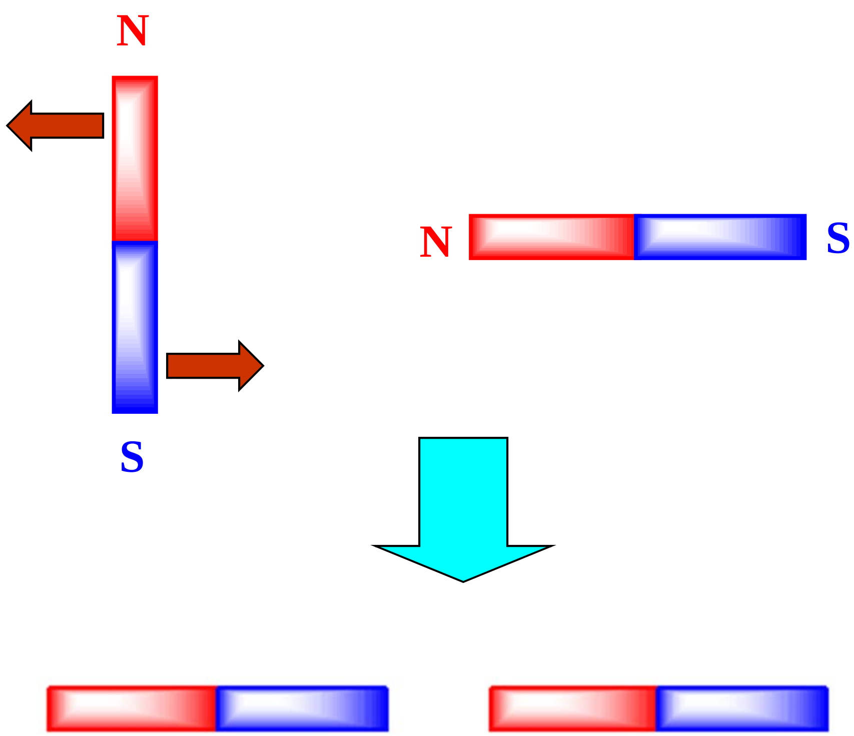
Bond Polarity

- bonding between unlike atoms results in ***unequal sharing of the electrons***
  - ✓ one atom pulls the electrons in the bond closer to its side
  - ✓ one end of the Bond has larger electron density than the other

→**Bond Polarity**

- ✓ the end with the larger electron density gets a partial negative charge (δ-) and the end that is electron deficient gets a partial positive charge (δ+)

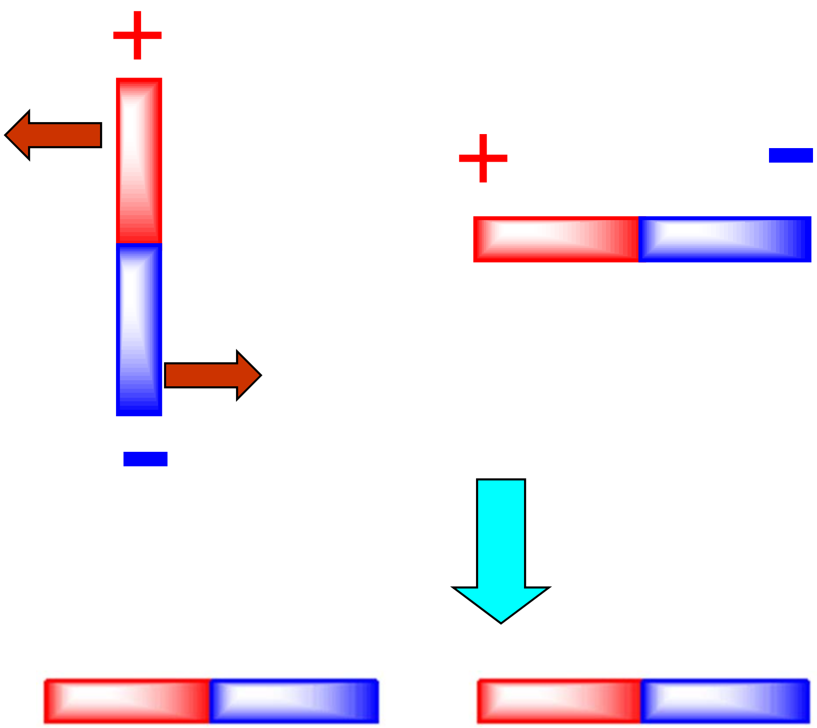
Why molecular polarity matters?



Recall how two magnets will interact when approach from an angle:

- The repulsion (same poles) and attraction (opposite poles) will cause the magnet to rotate
- After rotation, the two magnets will attract to each other

Polar molecules attract each other



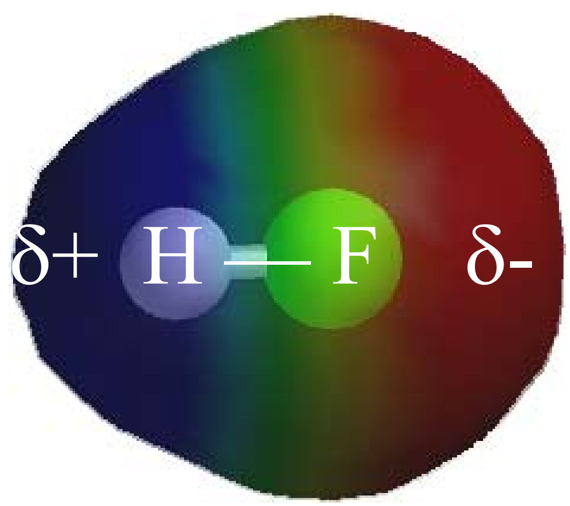
- Polar molecules can be attracted to each other like magnets:
- The repulsion (same charge) and attraction (opposite charges) will cause the molecule to rotate
- After rotation, the two molecules will attract to each other

Electronegativity

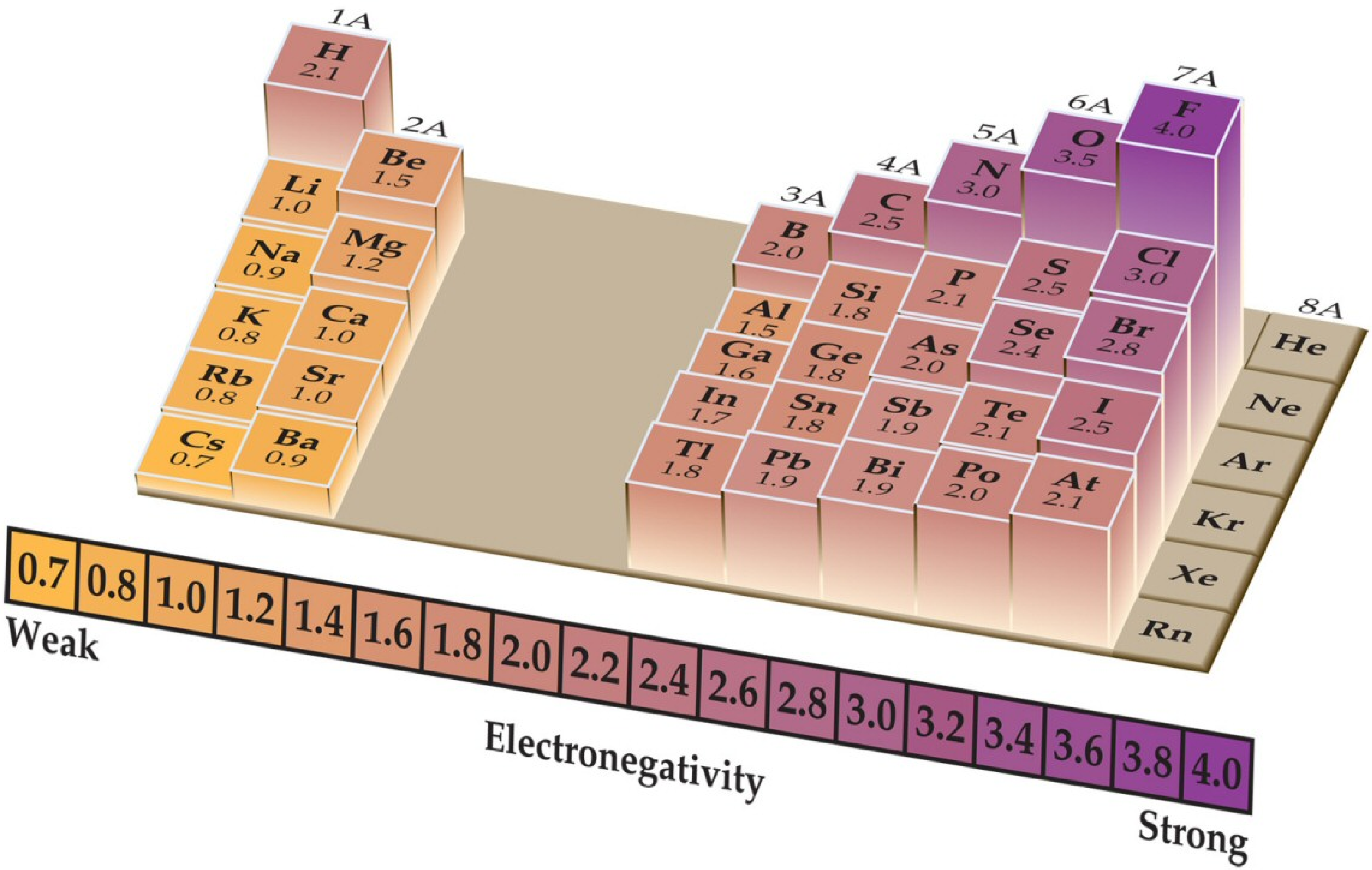
- Measure of the pull an atom has on bonding electrons
- increases across period (left to right)
- decreases down group (top to bottom)

→ Bond polarity: larger difference in electronegativity, more polar the bond

  - ✓ negative end toward more electronegative atom



Electronegativity: Main group



Electronegativity (EN) & Bond Polarity

Based on difference in EN between bonded atoms (ΔEN)

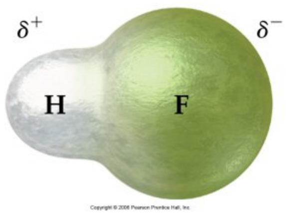
- **Pure covalent bond:** If ΔEN = 0. *Example: H-H in H_2*
- **Nonpolar covalent** bond**:** If ΔEN = 0.1~0.3, *Example: C-H in CH_4*
- **Polar covalent** bond: If ΔEN = 0.4 ~ 1.9. *Example: O-H in H_2O*
- **Ionic bond:** If ΔEN $\geq$ 2.0. *Example: O-Mg in MgO*

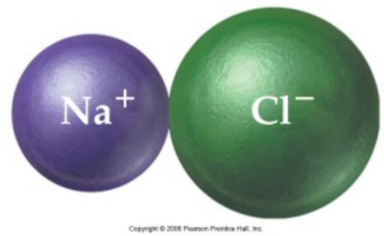
Bond Polarity

3.0-3.0
= 0.0

4.0-2.1
= 1.9

3.0-0.9
= 2.1





Covalent

Ionic

Non
polar

Polar

0

0.5

1.9

4.0

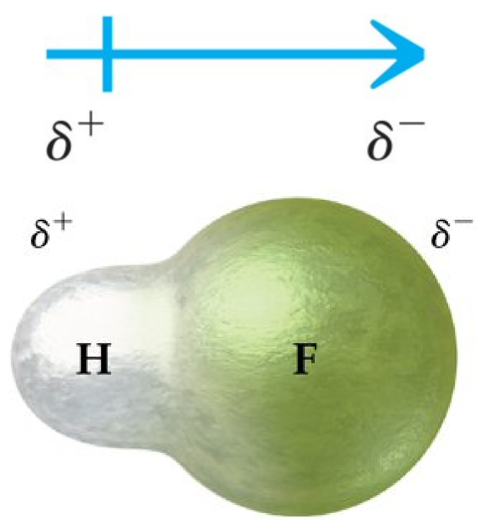
Electronegativity Difference

Bond Polarity: Dipole Moments

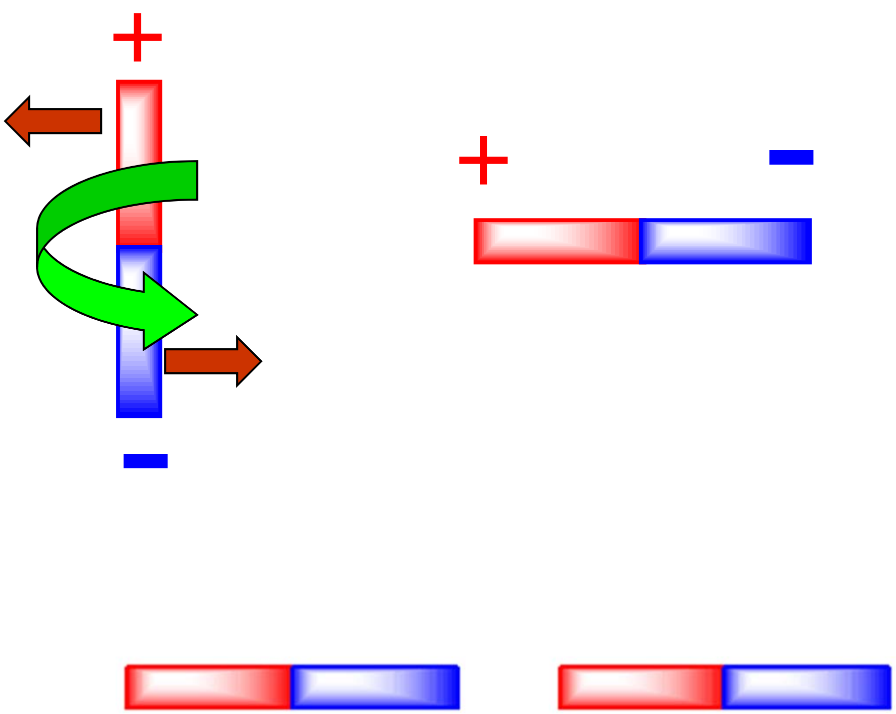
- Dipole: a material with positively and negatively charged ends

- Polar bonds or molecules have one end slightly positive, δ^+; and the other slightly negative, δ^-
  - ✓ not "full" charges, come from nonsymmetrical electron distribution

- Dipole Moment (μ) : a measure of the size of the polarity
  - ✓ measured in Debyes, D



Dipole Moment: *Torque produced by nearby electric charge*



Polar molecules can be attracted to each other like magnets:

- The repulsion (same charge) and attraction (opposite charges) leads to the torque that eventually will cause the molecule to rotate
- Higher charges on both ends of Polar molecules usually result in higher dipole moment

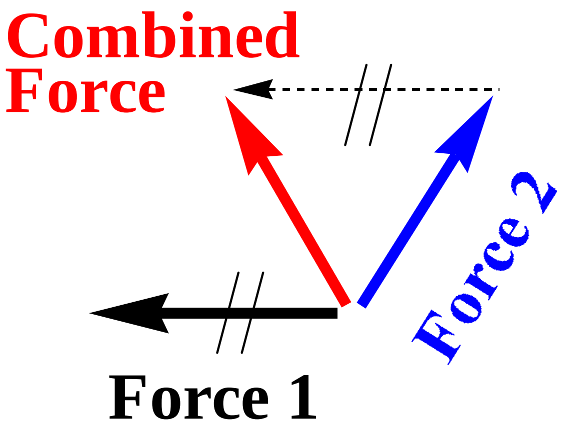
Polarity of Molecules

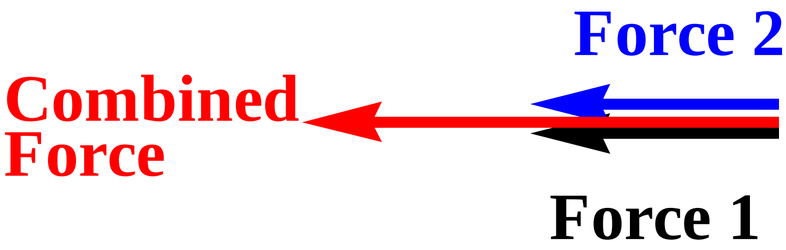
Polarity of molecule requires

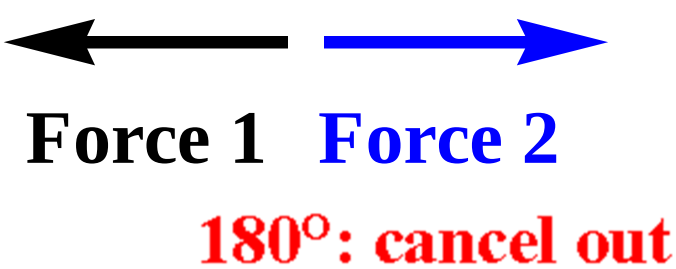
1) Polar bonds
    - electronegativity difference - theory
    - bond dipole moments - measured
2) Diatomic molecule: polar bond → polar molecule, e.g., HCl; nonpolar bond → nonpolar molecule (O_2)
3) Unsymmetrical shape so that Bond Polarity won't offset each other
    - **<u>Bent</u>** and **<u>Trigonal Pyramidal</u>** molecules are POLAR
    - vector addition

- Polarity affects the intermolecular forces of attraction

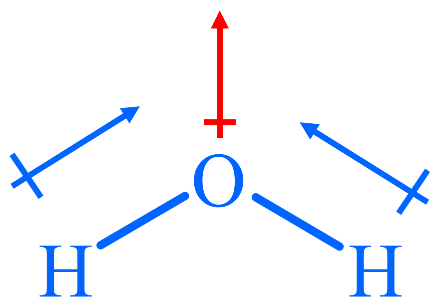
Bond Polarity vs. Molecular Polarity: Addition of Forces as Vector

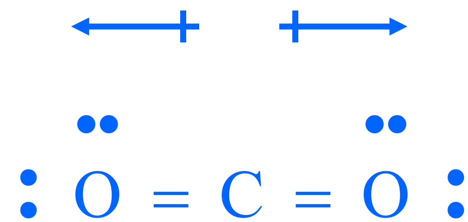






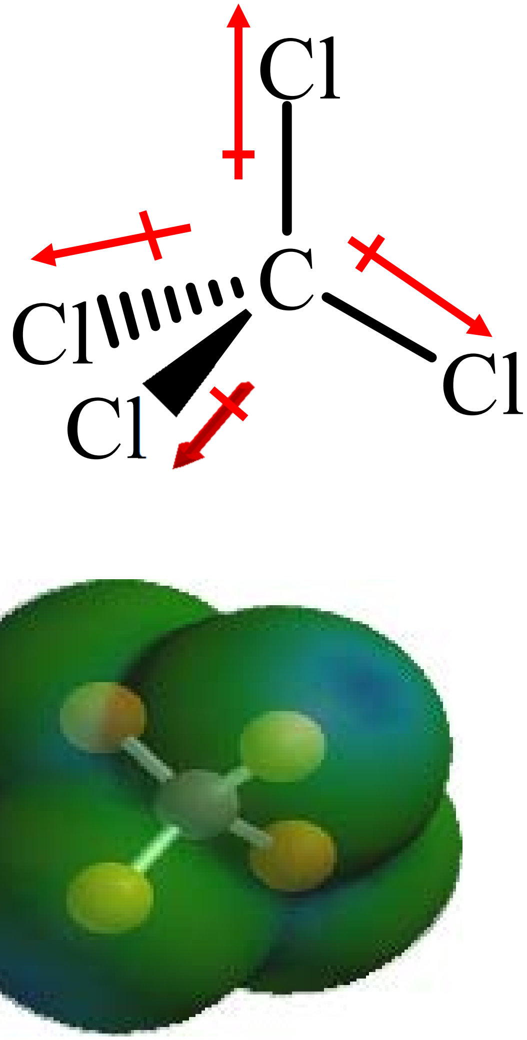
Polarity of Molecules:
Symmetry matters!



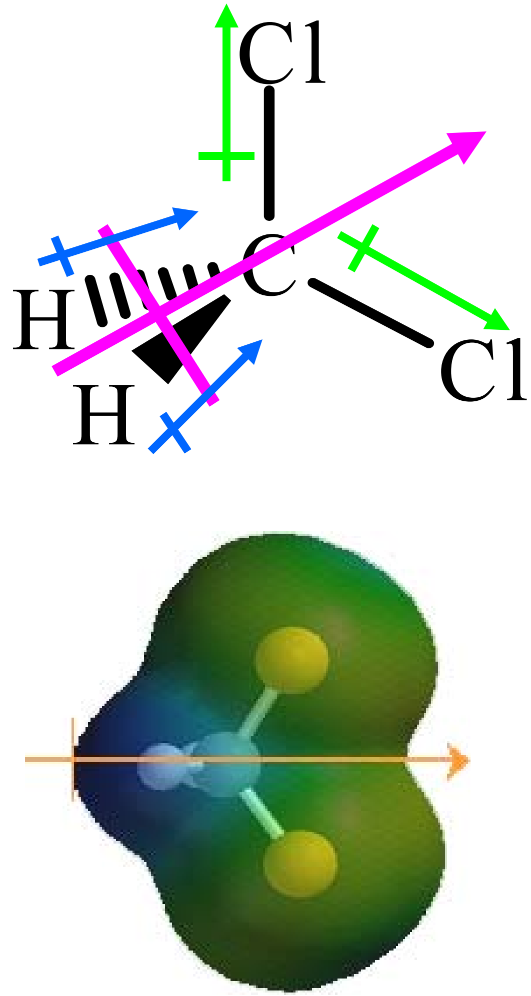


Polar bonds,
+ Unsymmetrical shape
→ water molecule as
POLAR

Polar bonds +
Symmetrical shape
→ ***polarity cancel***
→ CO2 molecule as
Nonpolar



CCl_4 : **NONPOLAR**



CH_2Cl_2: **POLAR**

Adding Dipole Moments

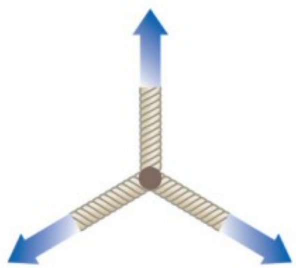
Nonpolar

Two identical polar bonds pointing in opposite directions will cancel. The molecule is nonpolar.

Polar

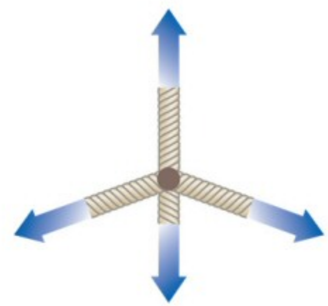
Two polar bonds with an angle of less than 180° between them will not cancel. The molecule is polar.

Nonpolar



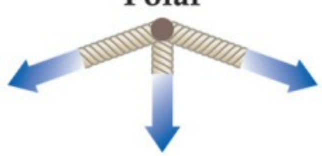
Three identical polar bonds at 120° from each other will cancel. The molecule is nonpolar.

Nonpolar



Four identical polar bonds in a tetrahedral arrangement (109.5° from each other) will cancel. The molecule is nonpolar.

Polar



Three polar bonds in a trigonal pyramidal arrangement (109.5°) will not cancel. The molecule is polar.

Note: In all cases where the polar bonds cancel, the bonds are assumed to be identical. If one or more of the bonds are different than the other(s), the bonds will not cancel and the molecule is polar.

Example:
Determine if NH_3 is Polar.

Information
Given: NH_3
Find: if Polar

- Design a Solution Map.

formula of compound → molecular polarity

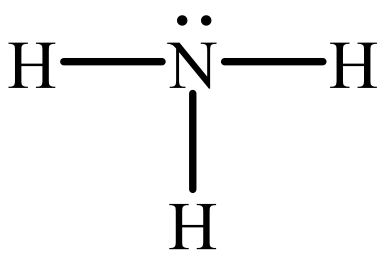
Lewis Structure

bond polarity & molecular shape

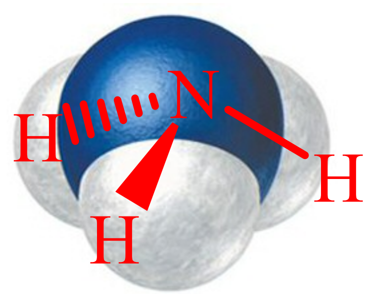
Example:
Determine if NH_3 is Polar.

Information
Given: NH_3
Find: if Polar
SM: formula → Lewis → Polarity & Shape → Molecule Polarity

- Apply the Solution Map.
  - ✓ Determine Shape of Molecule



4 areas of electrons around N;
3 bonding areas
1 lone pair



shape = trigonal pyramid

Example:
Determine if NH_3 is Polar.

Information

Given: NH_3

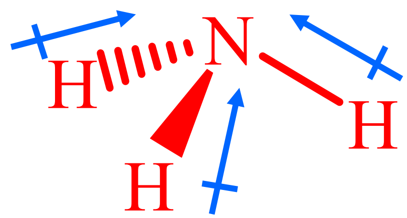
Find: if Polar

SM: formula → Lewis → Polarity & Shape → Molecule Polarity

- Apply the Solution Map.
  - ✓ Determine Molecular Polarity

bonds = polar

shape = trigonal pyramid

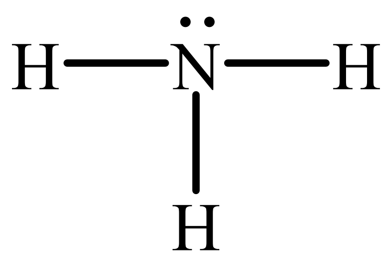


molecule = polar

Example:
Determine if NH_3 is Polar.

Information
Given: NH_3
Find: if Polar
SM: formula → Lewis → Polarity & Shape → Molecule Polarity

- Check.

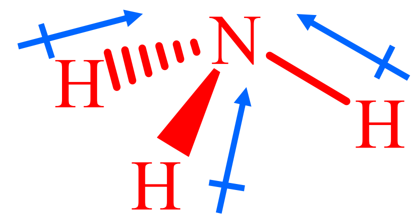


$N = 5$
$H = 3 \cdot 1$
total $NH_3 = 8$

bonding $= 3 \cdot 2\ e^-$
lone pairs $= 1 \cdot 2\ e^-$
total $NH_3 = 8\ e^-$

The Lewis structure is correct. The bonds are polar and the shape is unsymmetrical, so it should be polar.

bonds = polar
shape = trigonal pyramid



molecule = polar

How to Determine the Molecular Polarity

- Step 1: First, draw Lewis structure
- Step 2: use VSEPR theory to determine the molecular geometry/shape
- Step 3: consider the bond dipole moment addition.

Practice: Polar or Nonpolar?

- sulfur dioxide
- carbon tetrafluoride
- carbon disulfide
- hydrogen sulfide
- hydrogen bromide
- phosphorous trichloride
- sulfur dichloride
- $CHCl_3$
- CH_2O

Practice: Polar or Nonpolar?

Hint: molecular geometry

- sulfur dioxide — Bent
- carbon tetrafluoride — Tetrahedral
- carbon disulfide — Linear
- hydrogen sulfide — Bent
- hydrogen bromide — Single bond
- phosphorous trichloride — Trigonal pyramidal
- sulfur dichloride — Bent
- $CHCl_3$ — Tetrahedral
- CH_2O — Trigonal planar

Practice: Polar or Nonpolar?

- sulfur dioxide
- carbon tetrafluoride
- carbon disulfide
- hydrogen sulfide
- hydrogen bromide
- phosphorous trichloride
- sulfur dichloride
- $CHCl_3$
- CH_2O

- Polar
- Nonpolar
- Nonpolar
- Polar
- Polar
- Polar
- Polar
- Polar
- Polar