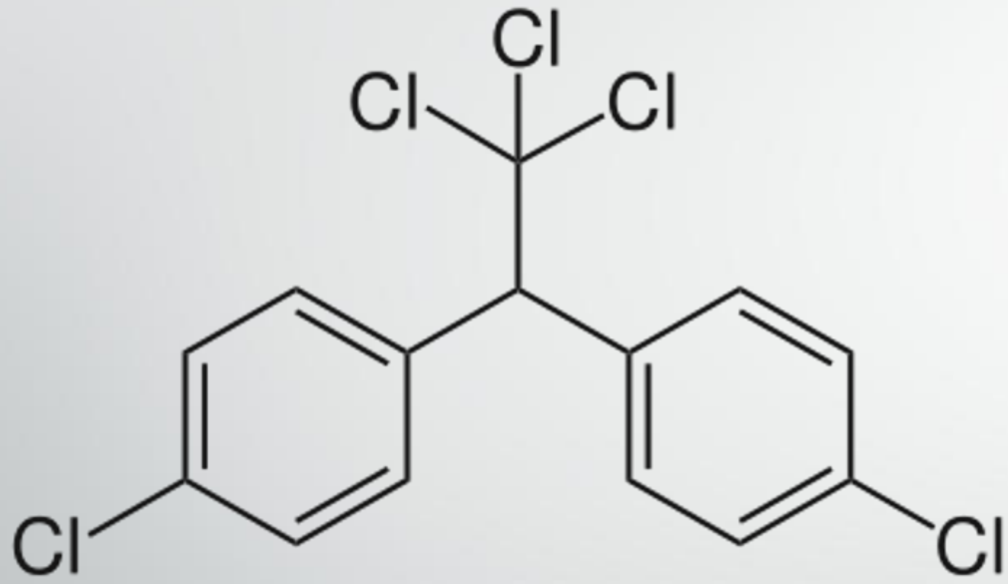
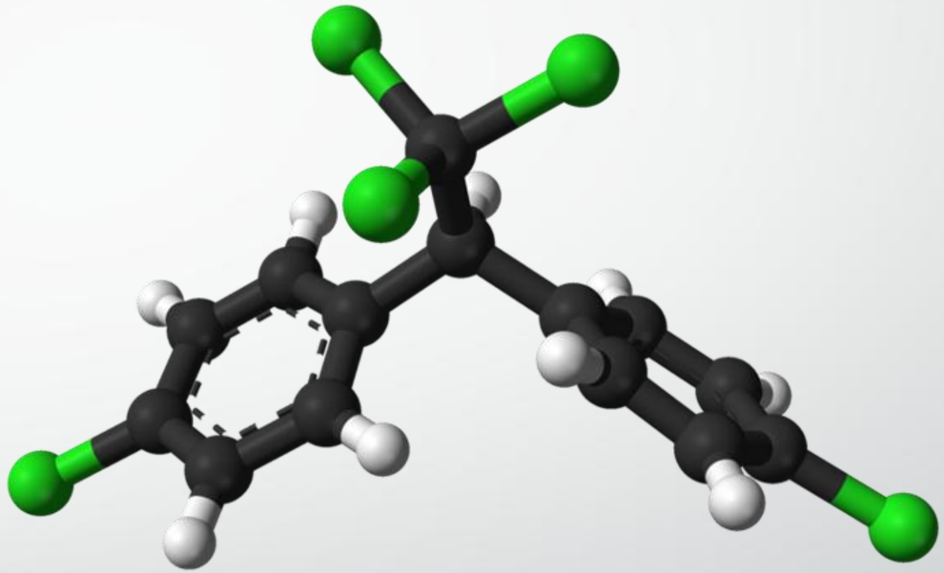
Molecular Structure And Properties





Auburn Mountainview

Karl Steffin, 2001

7/29/2026

By end of this unit I can…

- A.1 Create and/or evaluate models that illustrate how molecular properties influence the type(s) of intermolecular force(s) present in a substance.
- A.2 Create and/or evaluate a claim about the type(s), strength(s), and origin(s) of intermolecular forces present in a substance.
- B.1 Create and/or evaluate a claim that uses relative strength of intermolecular forces to explain trends in the physical properties of substances.
- C.1 Describe trends in properties of elements based on their position in the periodic table and the shell model of the atom.

By end of this unit I can…

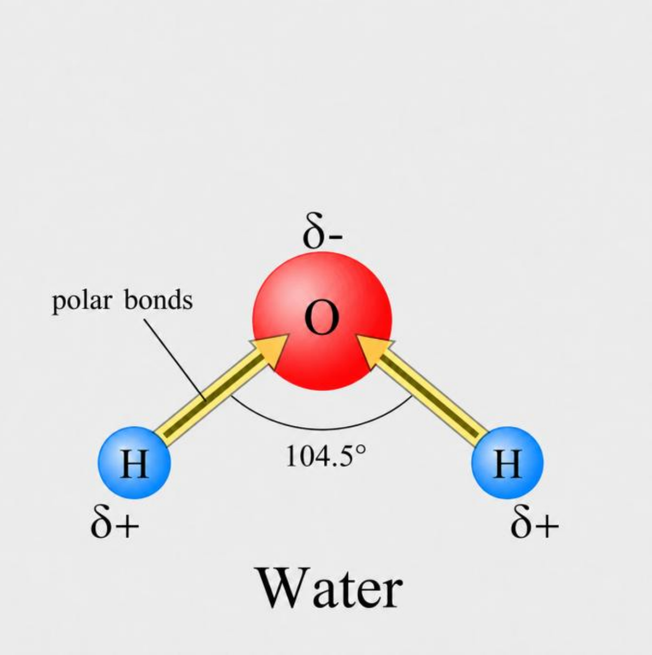
- D.1 Create and/or evaluate Lewis diagrams for molecular compounds and/or polyatomic ions.
- D.2 Determine if given molecules are structural isomers.
- E.1 Determine molecular geometry from a Lewis diagram using valence shell electron pair repulsion theory.
- F.1 Determine the polarity of a molecule from its molecular geometry and electron distribution.
- G.1 Create and/or evaluate a claim about the strength and type(s) of intermolecular forces present in a sample based on molecular polarity.

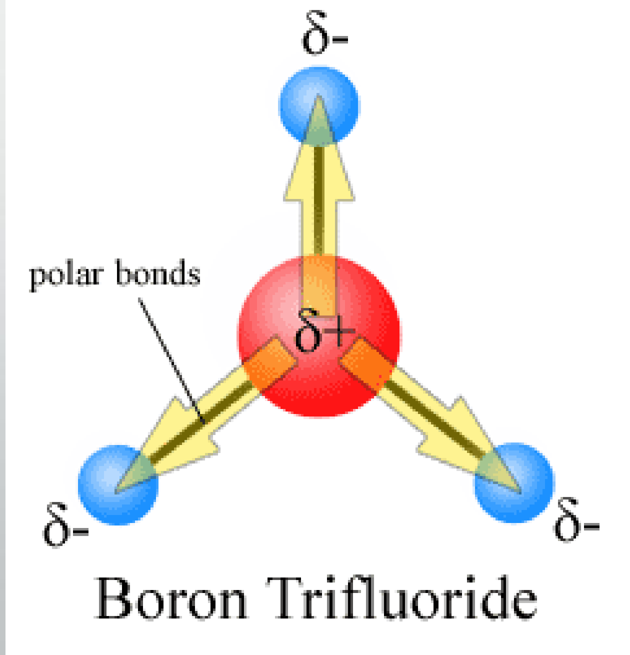
Basic Trends of the Periodic Table

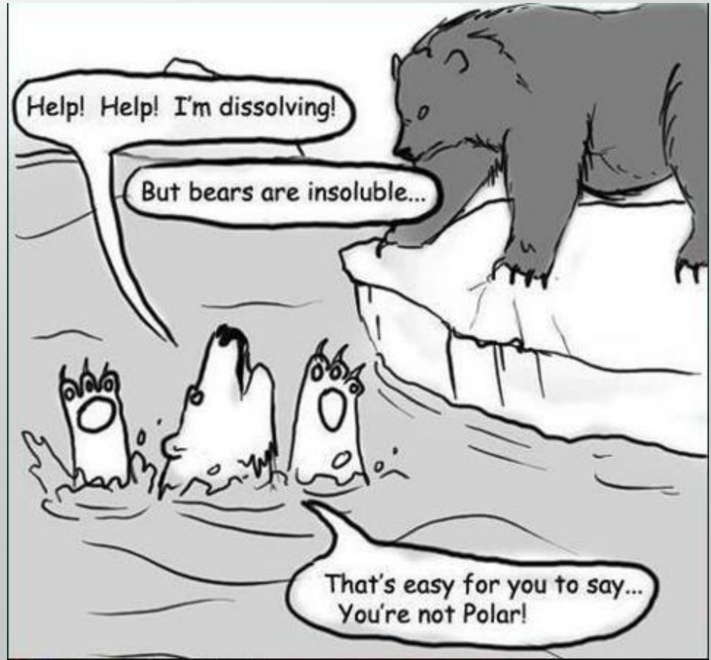
- Reactivity: Determined by valence electrons.
  - Valence: Number of electrons in the outer energy level (Row).
  - Most→ Metals: Family I, bottom. Nonmetals: Family VII, top.
- Atomic Radii: Distance from center of the atom to the outer electron.
  - Most→ Family I, bottom
- Electronegativity: Atom's ability to attract shared electrons towards itself.
  - Most→ Family VII, top

Electronegativity: Polarity

- Electrons are not always shared equally.
- Elements with greater electronegativity pull on electrons more.
- This causes molecules to be formed with a polarity (dipoles).
- In symmetrical molecules, dipoles can cancel.







Polarity chart

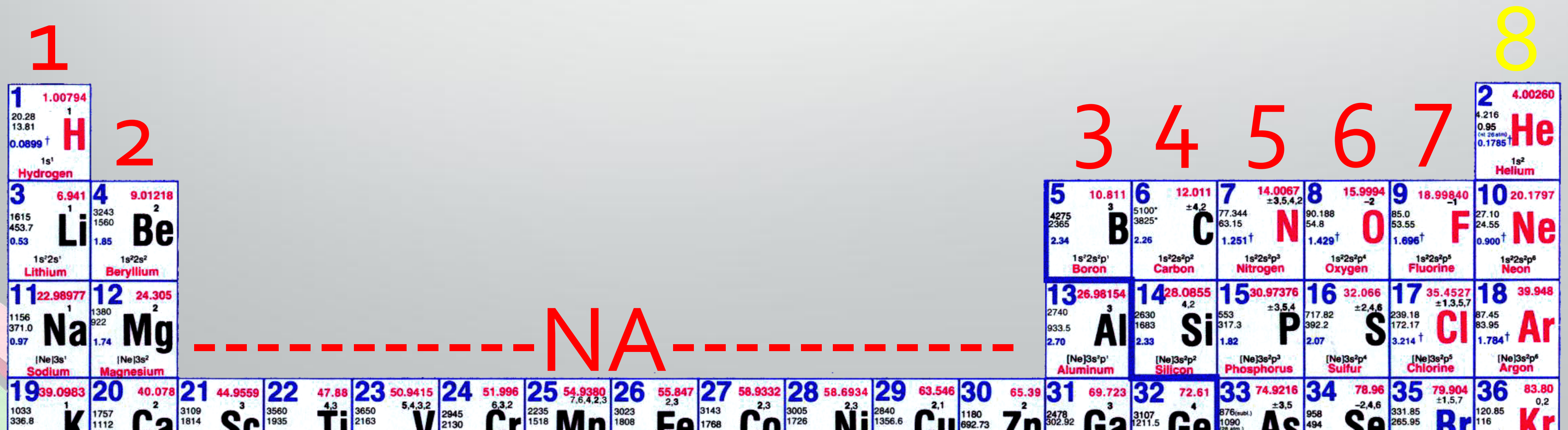
Electronegativity difference	Bond Type
$X \leq 0.4$	(Non-Polar) Covalent
$.4 \leftrightarrow 2.0$	Polar Covalent
$X \geq 2.0$	Completely Polar 'Ionic'

- Ex: HCl- Hydrogen: 2.20, Chlorine: 3.16
  - 3.16-2.20 = .96 (Polar Covalent)
- Ex: NO_2- Nitrogen: 3.04, Oxygen: 3.44
  - 3.44-3.04 = .40 (NP Covalent)
- Ex: NaCl- Sodium: .93, Chlorine: 3.16
  - 3.16-.93 = 2.23 (Completely Polar… Ionic)

Electronegativity (Pauling Scale)		
Z	Sym	Magnitude
1	H	2.2
2	He	
3	Li	0.98
4	Be	1.57
5	B	2.04
6	C	2.55
7	N	3.04
8	O	3.44
9	F	3.98
10	Ne	
11	Na	0.93
12	Mg	1.31
13	Al	1.61
14	Si	1.9
15	P	2.19
16	S	2.58
17	Cl	3.16
18	Ar	

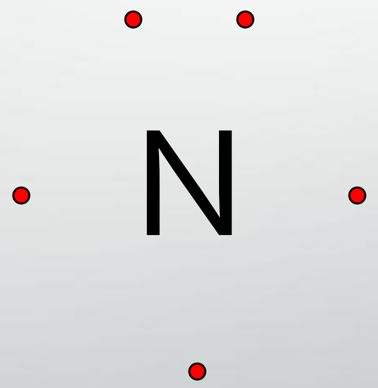
More about Electron's

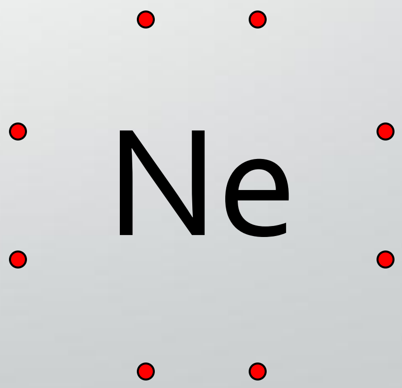
- A more simplified way to look at electrons is to look at their Lewis Dot Structures.
- This counts the atoms valence electrons
  - This relates directly to the family #
  - Nobel gasses: Helium only has 2 outer electrons.



Lewis Dot Structures

- **Magnesium: [Mg] Family II.**
- **Nitrogen: [N] Family V.**
- **Neon: [Ne] Family VIII.**





Rule 1: 1 e^- side first.

Rule 2: Balanced sides if possible.

Rule 3: Max 2e^- per side.

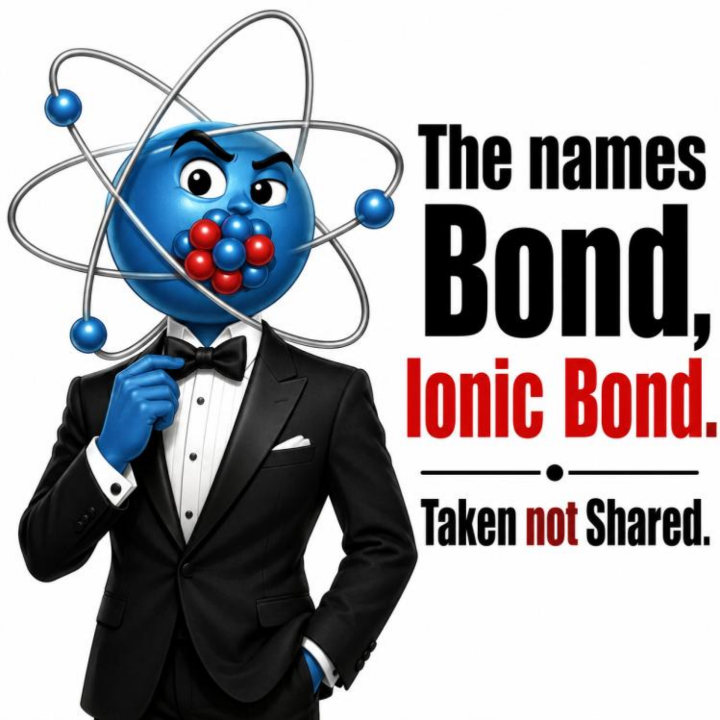
For Nobel Gasses… Draw a complete shell

Bonding

- Bonding is the process of two or more atoms joining chemically to form a new product. All atoms want complete energy levels (octet rule).
- Bonding is very common and has three forms:
  - Ionic, Covalent and Metallic.

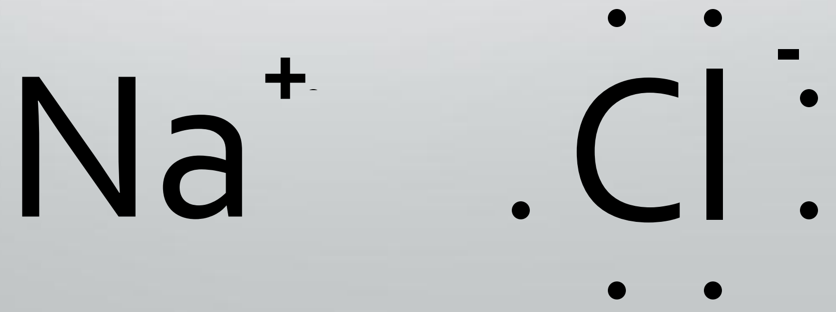
Ionic Bonding

- Ionic bonding involves positive ions joining negative ions.
- Looking at the periodic table positive ions are on the left and negative ions on the right.
- So… Ionic bonding: metal/non-metal's bonding.
    - Electronegativity (2.0+)



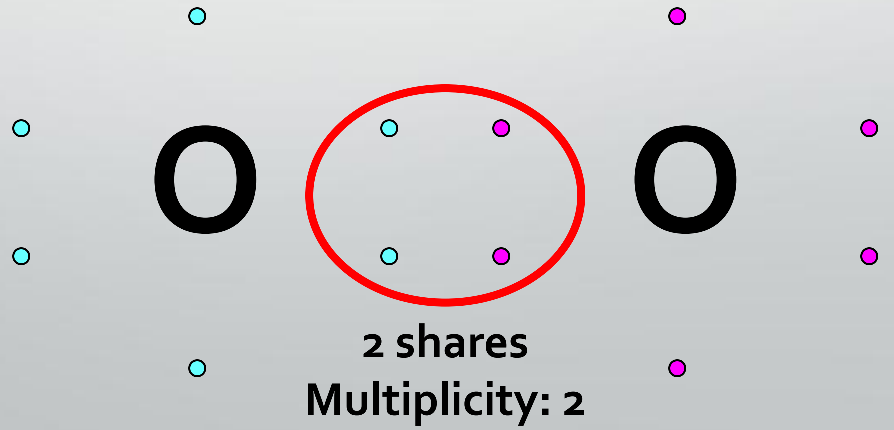
Why Ionic Bonds Happen

- Look at a common ionic bond: NaCl.
  - Draw The Lewis Structure for Na and Cl.
  - Cl is missing 1, Na has 1 extra. Na gives up 1.
  - The metal Na+ ion and non-metal Cl- ion attract.
- Completing Energy levels makes this is a very strong bond.



Covalent Bonding

- Sharing electrons to complete the octet rule.
- This happens when an atom needs one to three electrons to be complete. (Fam: 5-7)
  - Looking at the periodic table, these elements are non-metals.
- Covalent Bonding is non-metal/non-metal bonding.
  - Electronegativity (Nonpolar: 0-.4, Polar: .4 ↔ 2.0)



Molecular Shapes

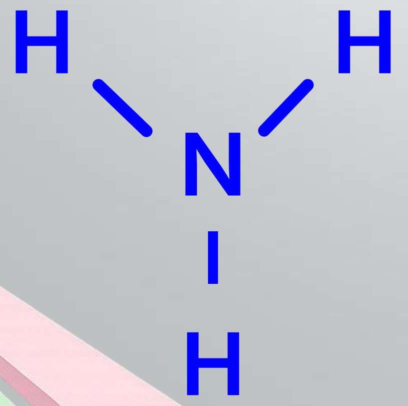
- Depending on how individual elements bond to each other also determines their molecular shape.
- For two elements/atoms bonded together there is only one shape: Linear.

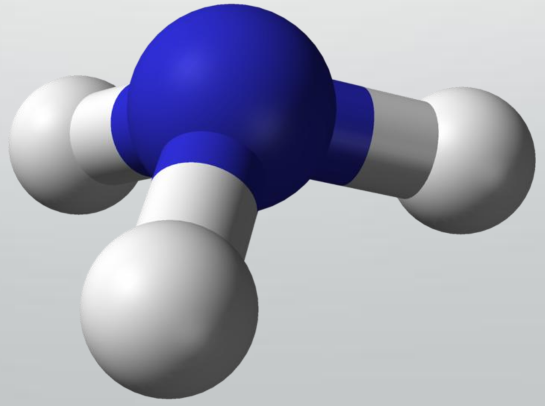
$$F_2 \longrightarrow F - F$$

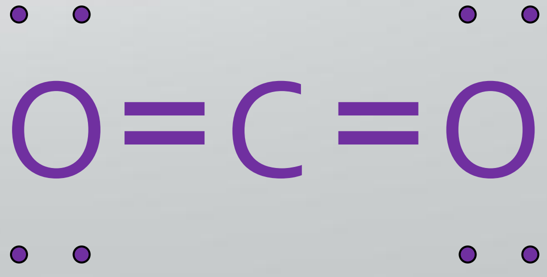
- More complicated shapes are formed when multiple elements/atoms bond.

VSEPR Theory

- When covalent bonds are formed they create slight charges (remember electrons want to repel).
- The Valence Shell Electron Pair Repulsion Theory helps to determine the shape of these molecules.
- Here is shown the structural model and the stick and ball model of Ammonia (NH_3). Lewis Diagrams (CO_2) include unpaired electrons.







Algorithm to Solve VSEPR Shapes

- Pairs of electrons that surround the central atom of a molecule or ion are arranged as far apart as possible to minimize repulsion.
- To predict the shapes of molecules, follow these steps:

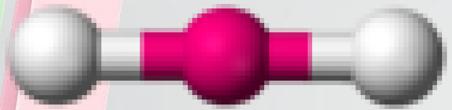
1. Decide which is the central atom in a molecule (most electronegative)
2. Count the valence electrons around the central atom.
3. Count the electrons needed by the outer atom(s) to become complete.

VSEPR Algorithm cont.

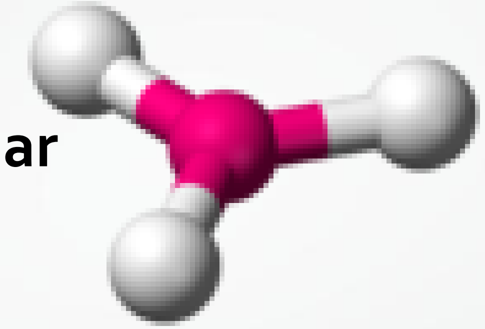
1. Add the numbers in step 2 + 3 then divide by two to get the Valence Shell Electron Pair (VSEP) number.
   - If step 3 requires more than one bond (Outer element is Family 4-6.); subtract one from the VSEP count for each extra bond beyond the first.
2. This VESP number is the Basic Shape.
3. Using the number in step 3 cross out that many electrons around the central atom. (cross out single electron first)
   - Circle any pairs still remaining.
   - These are called Lone Pairs and will warp the Native Shape.
4. Look at the VSEP chart to find the new warped shape.
5. Draw a model of the molecule.

Basic VSEPR Predictions

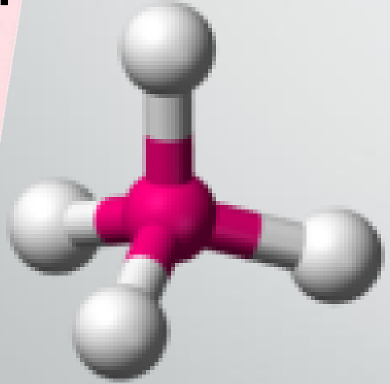
2 Linear

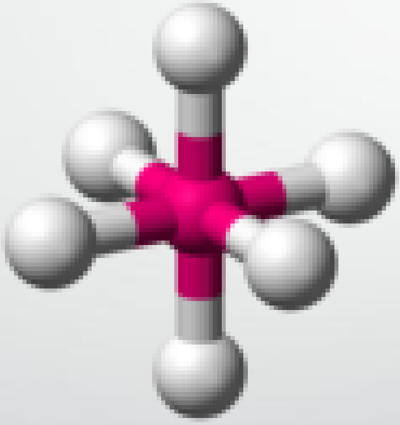


3 Trigonal Planar

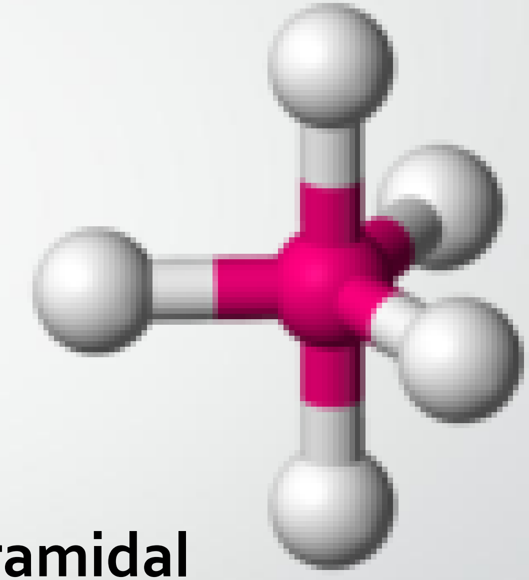


4 Tetrahedral

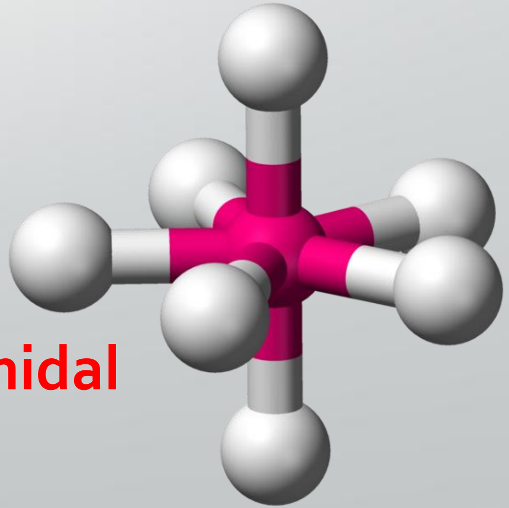




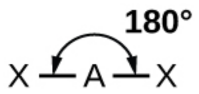
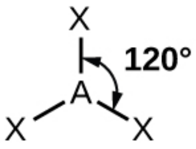
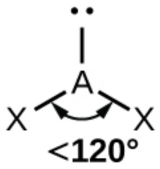
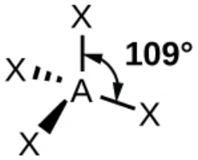
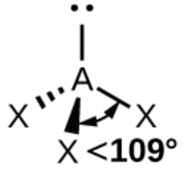
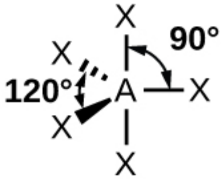
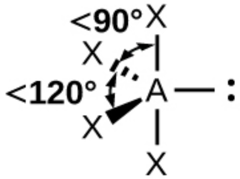
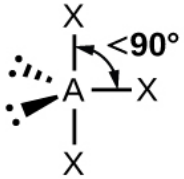
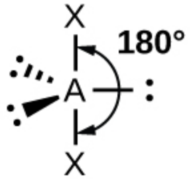
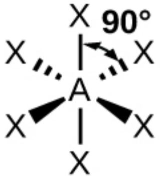
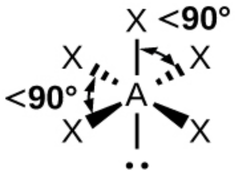
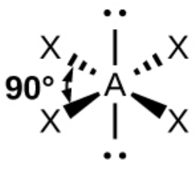
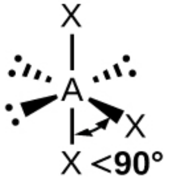
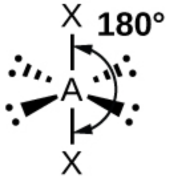
6 Octahedral

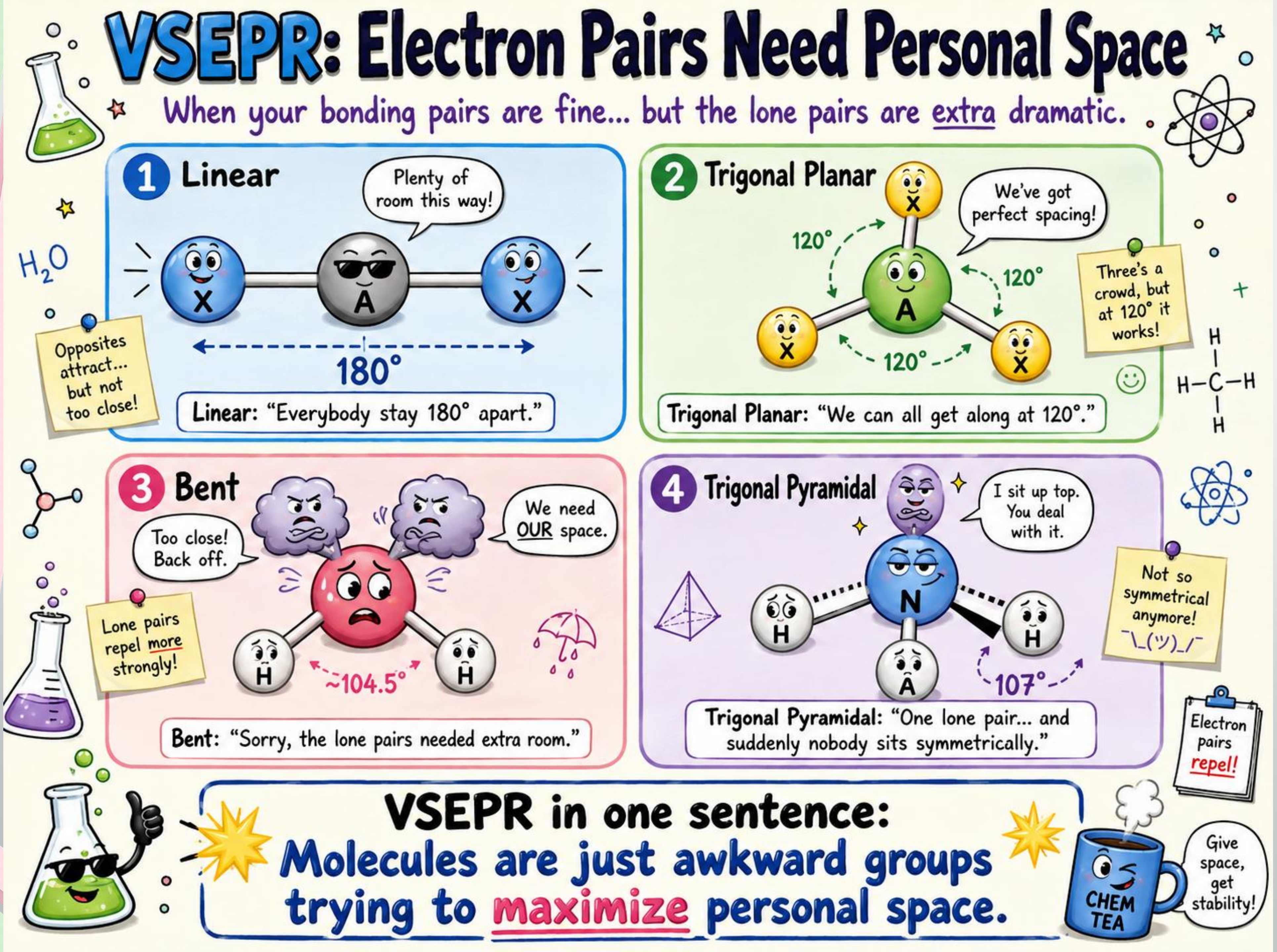


5 Trigonal Bipyramidal



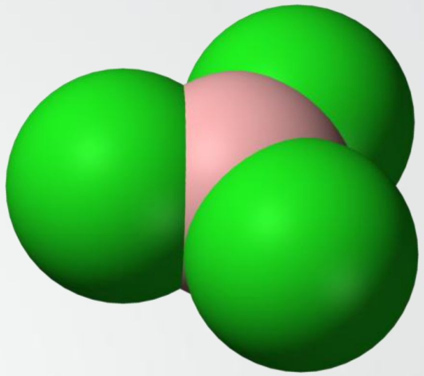
7 Pentagonal Bipyramidal

Number of electron pairs	Electron pair geometries: 0 lone pair	1 lone pair	2 lone pairs	3 lone pairs	4 lone pairs
2	 Linear				
3	 Trigonal planar	 Bent or angular			
4	 Tetrahedral	 Trigonal pyramid	 Bent or angular		
5	 Trigonal bipyramid	 Sawhorse or seesaw	 T-shape	 Linear	
6	 Octahedral	 Square pyramid	 Square planar	 T-shape	 Linear



VSEPR: Electron Pairs Need Personal Space
When your bonding pairs are fine... but the lone pairs are extra dramatic.
1 Linear
Plenty of room this way!
X
A
X
180°
Linear: "Everybody stay 180° apart."
Opposites attract... but not too close!
H2O
2 Trigonal Planar
We've got perfect spacing!
X
A
X
X
120°
120°
120°
Trigonal Planar: "We can all get along at 120°."
Three's a crowd, but at 120° it works!
H
H—C—H
H
3 Bent
Too close! Back off.
We need OUR space.
H
H
~104.5°
Bent: "Sorry, the lone pairs needed extra room."
Lone pairs repel more strongly!
4 Trigonal Pyramidal
I sit up top. You deal with it.
N
H
H
A
107°
Trigonal Pyramidal: "One lone pair... and suddenly nobody sits symmetrically."
Not so symmetrical anymore! ¯_(ツ)_/¯
Electron pairs repel!
VSEPR in one sentence:
Molecules are just awkward groups trying to maximize personal space.
CHEM TEA
Give space, get stability!

Example



- BCl_3
- 1. Central Atom: B

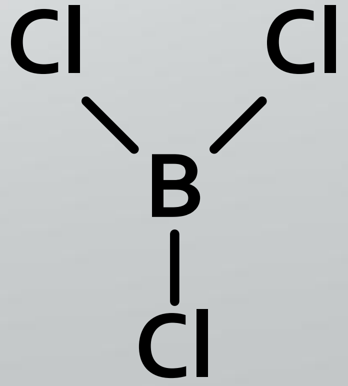
2. B Valence: 3, 3. Cl Needed: 1 x 3

4. 3 + 1 x 3 = 6 / 2 = 3

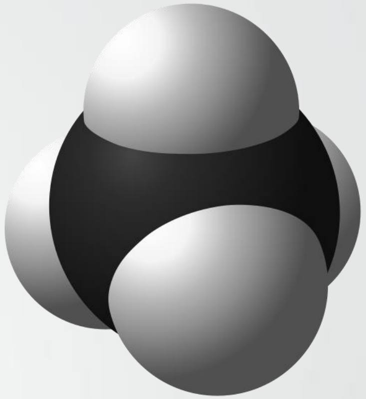
5. Basic Shape: Trigonal Planar

6. Cross out 1 x 3 around Boron. Circle pairs (o).

7. The basic shape holds… Trigonal Planar

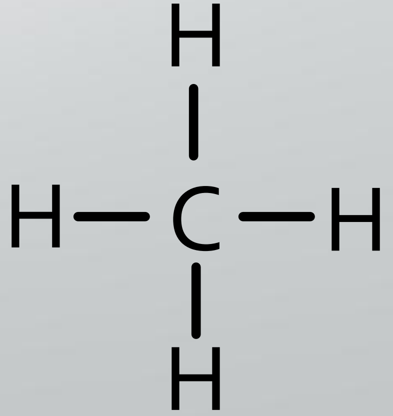


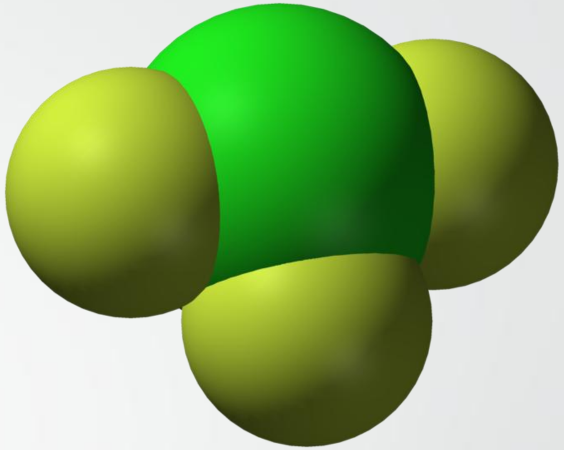
Example



- CH_4
- Central Atom: C

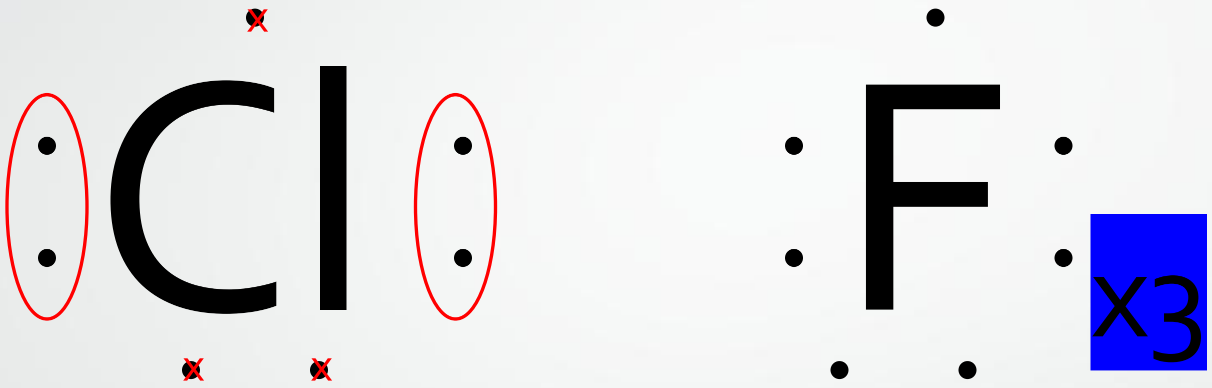
- C Valence: 4,   H Needed: 1 x 4
- 4 + 1 x 4 = 8 / 2 = 4
- 4 Basic Shape: Tetrahedral
- Cross out 1 x 4 around Carbon. Circle pairs (o).
- The basic shape holds… Tetrahedral



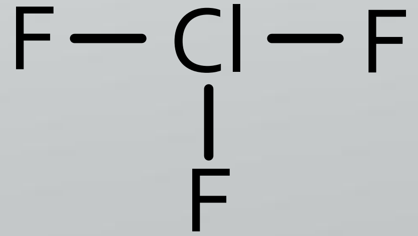


Example

- ClF_3
- Central Atom: Cl

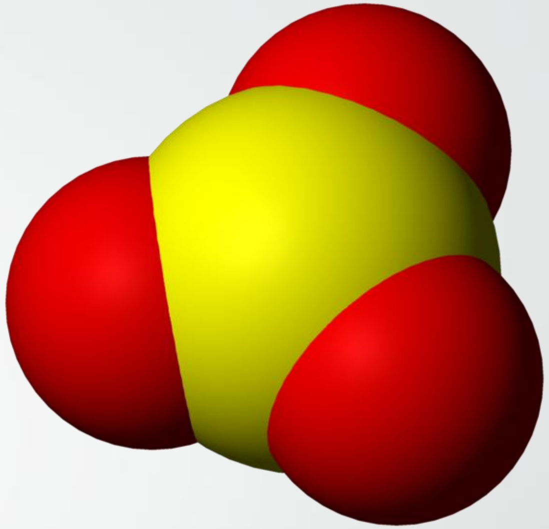


- Cl Valence: 7, F Needed: 1 x 3
- 7 + 1 x 3 = 10 / 2 = 5
- 5 Basic Shape: Trigonal Bipyramidal
- Cross out 1 x 3 around Chlorine. Circle pairs (2).
- The basic shape warps… T Shaped



Multiple Bonds (Outer Elements)

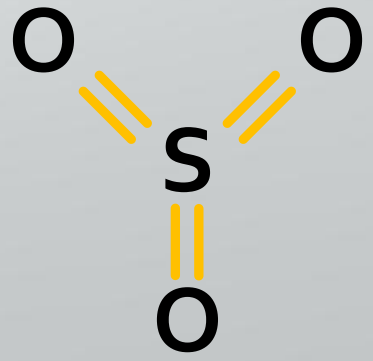
- Some elements need to have more than a single bond when not the central atom.
  - Oxygen (Family VI) creates double bonds (multiplicity 2). $=$
  - Nitrogen (Family V) creates triple bonds (multiplicity 3). $\equiv$
- When doing VSEP math after dividing by two then…
  - Subtract 1 from the total for every additional bond.
  - This new number is the Basic Shape.

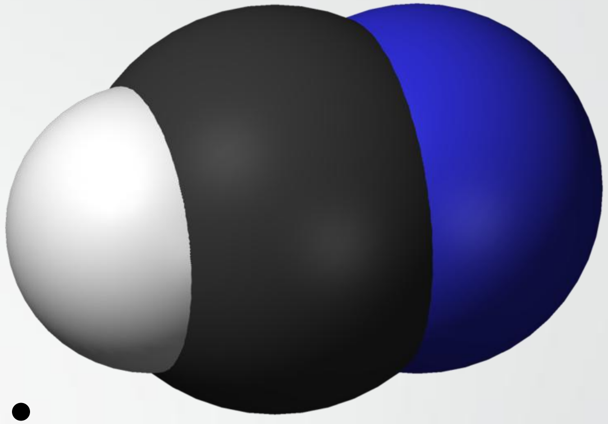


Example

- SO_3
- Central Atom: S

- S Valence: 6,   O Needed: 2 x 3
-         6 + 2 x 3 = 12 / 2 = 6 - (2-1) x 3 = 3
- 3 Basic Shape: Trigonal Planar
- Cross out 2 x 3 around Sulfur. Circle pairs (o).
- The basic shape holds… Trigonal Planar





Example

- HCN
- Central Atom: C

- C Valence: 4, H Needed: 1 x 1 N Needed: 3 x 1
- 4 + 1 x 1 + 3 x 1= 8 / 2 = 4 - (1-1)x1 - (3-1)x1= 2
- 2 Basic Shape: Linear
- Cross out 1 + 3 around Carbon. Circle pairs (o).
- The basic shape holds… Linear

H—C≡N

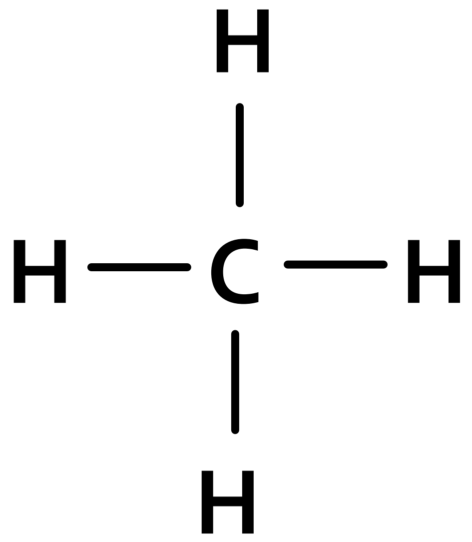
Lewis Diagrams

1. Count Valence Electrons including anions and cations.
2. Identify the central atom.
   - Draw Single Bonds to each outer atom.
3. Fulfill Outer Octets (2 for H).
4. Complete Central Octets
   - If the central atom lacks an octet, convert lone pairs from outer atoms into double or triple bonds.

CH_4

$4+1+1+1+1=8$

$-8 = 0$

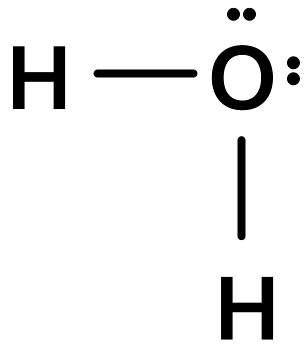


H_2O

$1+1+6=8$

$-4 = 4$

$-4 = 0$

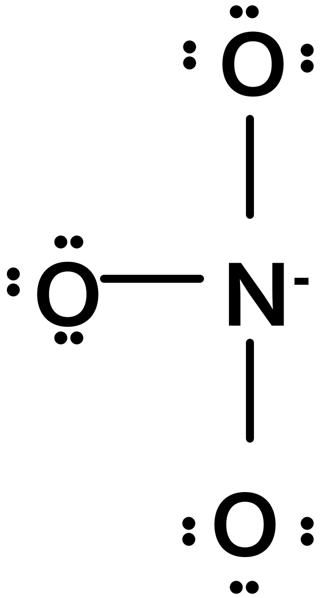


NO_3^-

$5+6+6+6+1=24$

$-6 = 18$

$-18 = 0$

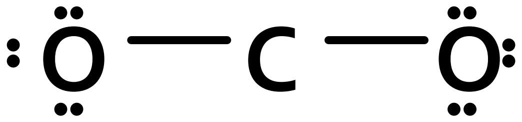


CO_2

$4+6+6=16$

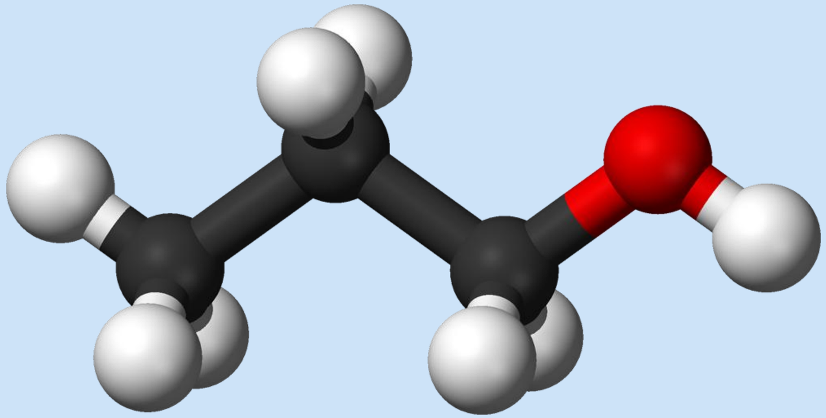
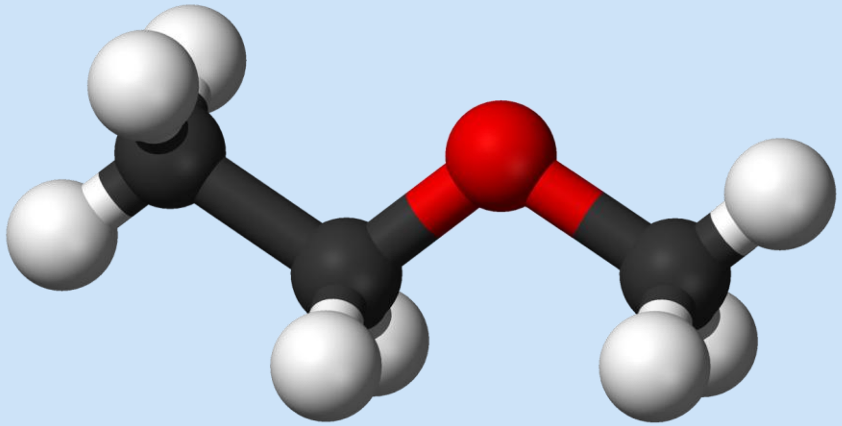
$-4 = 12$

$-12 = 0$



Isomers

- Iso (same), Mer (part): Molecule with same formula but different structure
  - Common in polymers (repeating molecules).

Propanol (C_3H_8O)	Methoxyethane (C_3H_8O)
 Used to treat high blood pressure & anxiety (β Blocker).	 Used in expirments as an organic solvent.

Structural Models in Organic Chemistry

- **When looking at complex molecules, shortcuts are used.**
  - Carbon and Hydrogen are ‘missing’

n-Butylamine: $CH_3(CH_2)_3NH_2$ 	Benzene: C_6H_6