

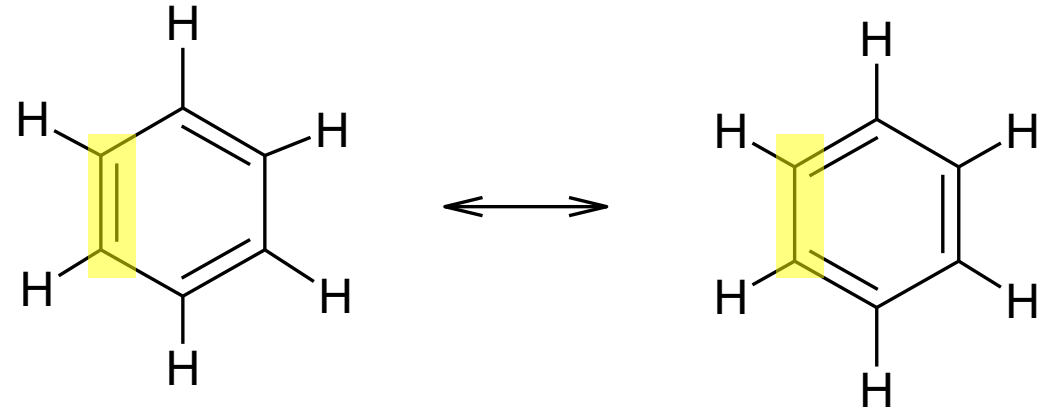
N₂O – Bonding

Formal Charge and VSEPR

Resonance

When more than one valid Lewis structure can be written for a molecule.

Example:
Benzene, C_6H_6

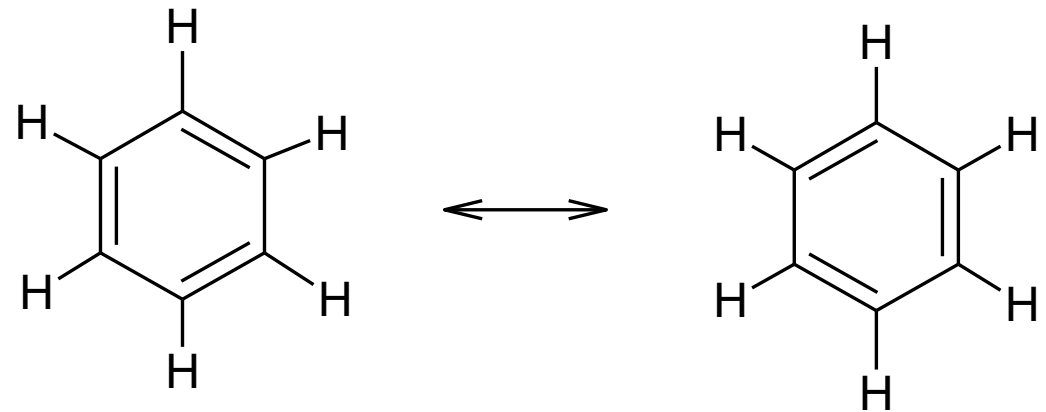


- You would expect the single bonds to be longer than the double bonds. But when measured the bond lengths in the ring are identical! The lengths of all the bonds are between a single and double bonds.
- The actual structure is an average of the resonance structures.

Resonance Bond Length and Energy

Resonance bonds are shorter and stronger than single bonds.

Resonance bonds are longer and weaker than double bonds.

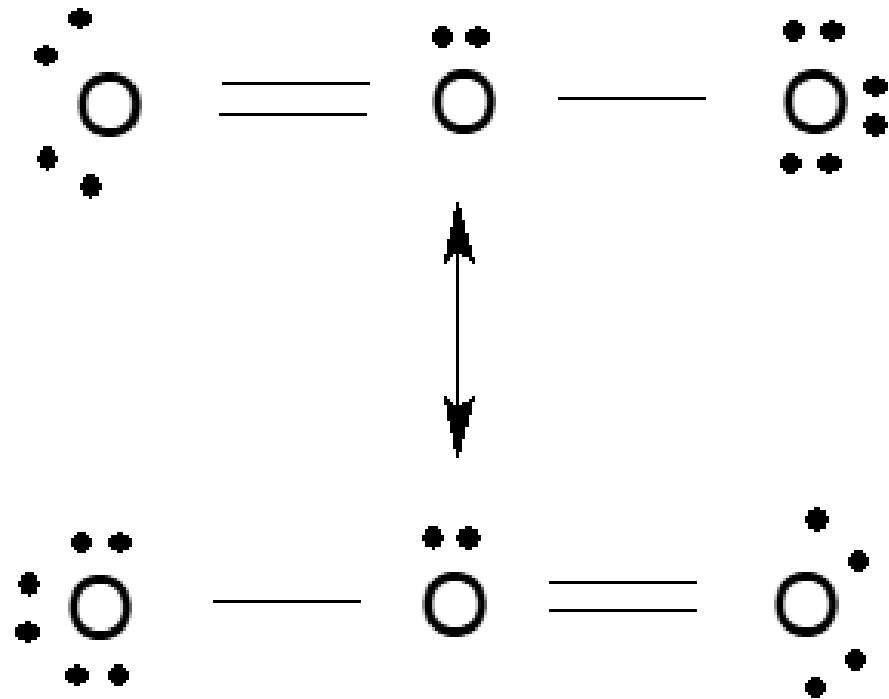


Resonance in Ozone, O₃

Neither structure is correct!

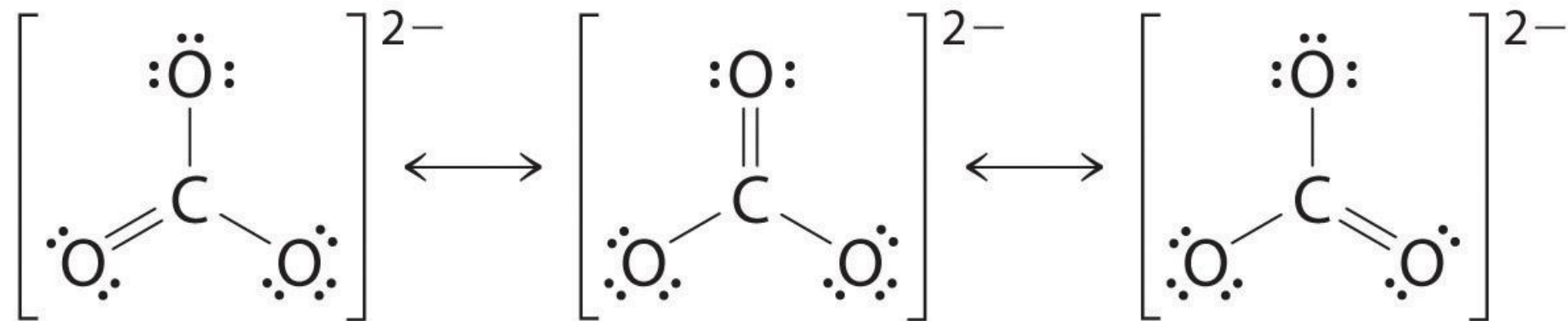
Oxygen bond lengths are identical, and intermediate to single and double bonds.

We know this from experimental data!

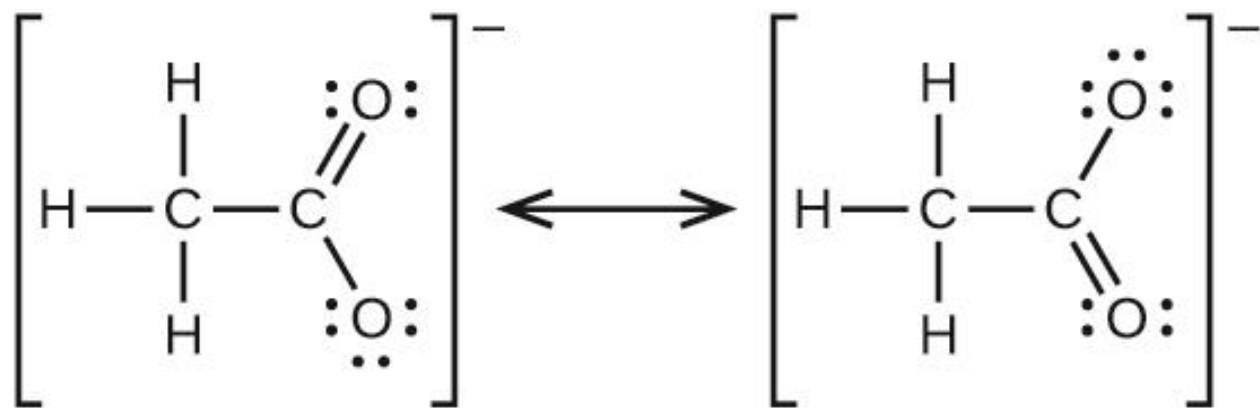


Resonance in Polyatomic Ions

Resonance in a carbonate ion:



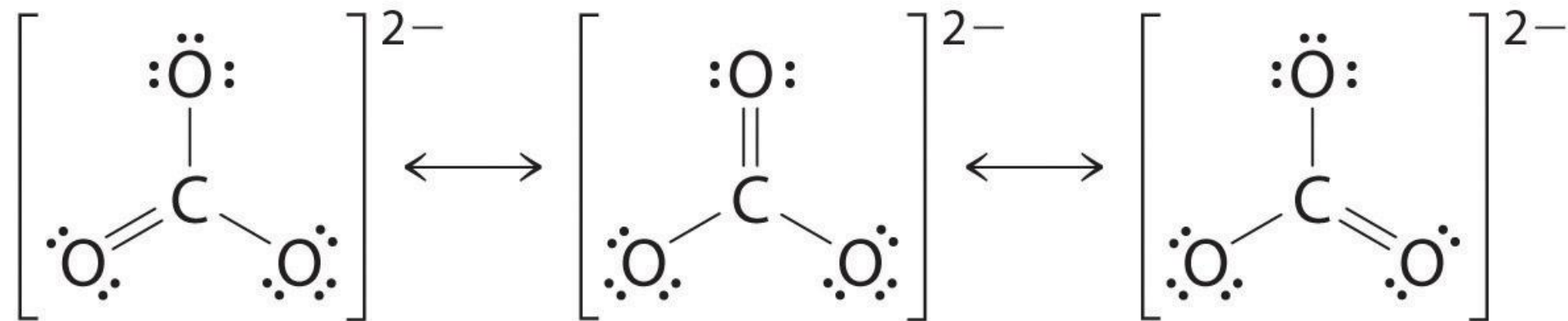
Resonance in an acetate ion:



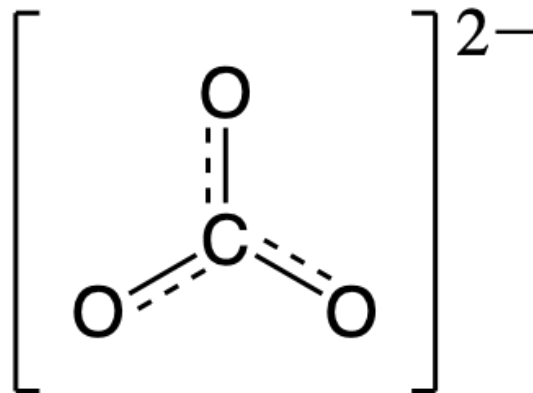
Use square brackets and double headed arrows between resonance structures!

Resonance in Polyatomic Ions

Resonance in a carbonate ion:



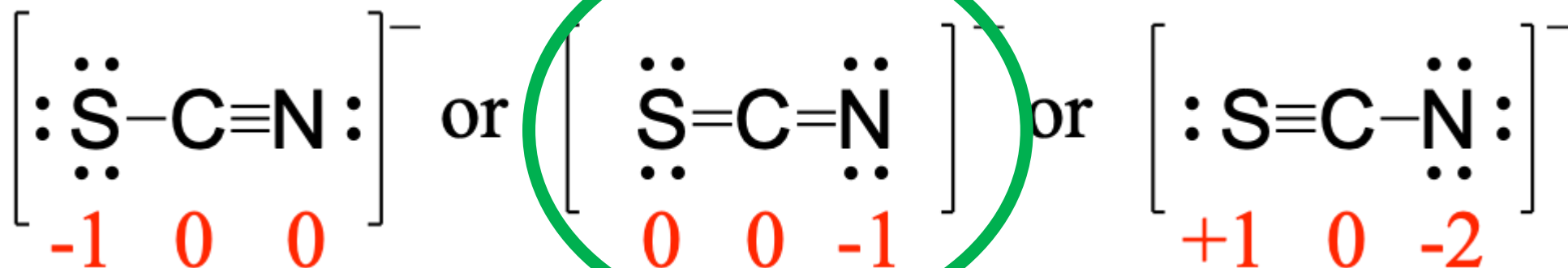
Sometimes see it drawn with a dashed line to represent a combo of all the resonance structures:



Formal Charge

Some resonance structures are “better,” more stable, more common than others.

Minimizing the “formal charge” on the atoms, and having negative formal charge on the more electronegative elements helps predict which structure is preferred.



How to Calculate Formal Charge

Formal Charge = **Should** - **Has**

$$\# \text{ of Valence } e^- - \left(\# \text{ lone pairs on the atom} + \frac{1}{2} \text{ the } \# \text{ of bonded } e^- \right)$$

Half because they are sharing with the other atom

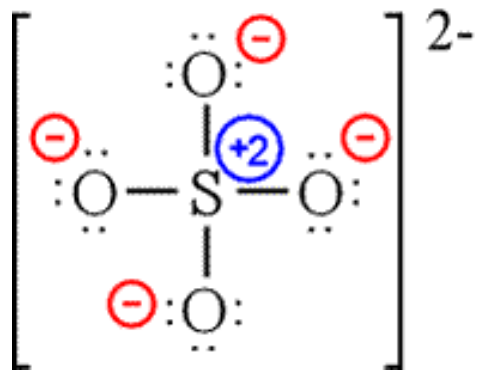
How to Calculate Formal Charge

Some guidelines:

- Atoms would like a FC as close to 0 as possible.
- Any negative FC should be on the most electronegative atoms.
- The sum of all FC must equal the overall charge on the ion or molecule.

Ex: Sulfate Ion

$$\text{FC} = \# \text{ of Valence } e^- - \# \text{ lone pairs on the atom} - \frac{1}{2} \text{ the } \# \text{ of bonded } e^-$$



Each Oxygen:

$$(6) - (6) - \frac{1}{2} (2) = -1$$

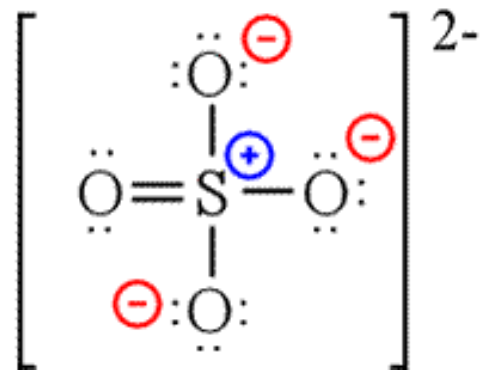
Sulfur:

$$(6) - (0) - \frac{1}{2} (8) = +2$$

Sum

$$4 (-1) + (+2) = -2$$

Good, that matches the charge on the sulfate ion!



Single Bonded Oxygens

$$(6) - (6) - \frac{1}{2} (2) = -1$$

Double Bonded Oxygen:

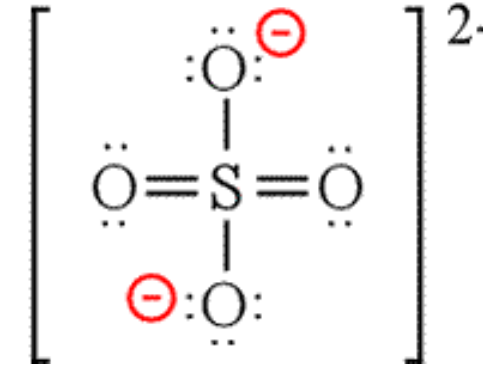
$$(6) - (4) - \frac{1}{2} (4) = 0$$

Sulfur:

$$(6) - (0) - \frac{1}{2} (10) = +1$$

Sum

$$3 (-1) + (0) + (+1) = -2$$



Single Bonded Oxygen:

$$(6) - (6) - \frac{1}{2} (2) = -1$$

Double Bonded Oxygens:

$$(6) - (4) - \frac{1}{2} (4) = 0$$

Sulfur:

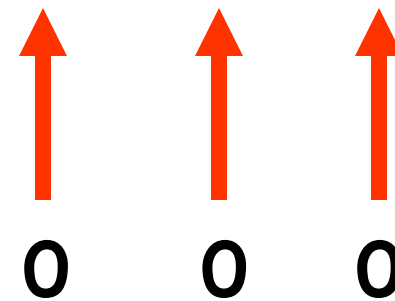
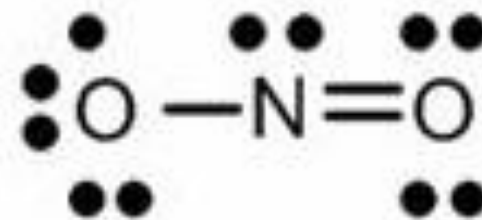
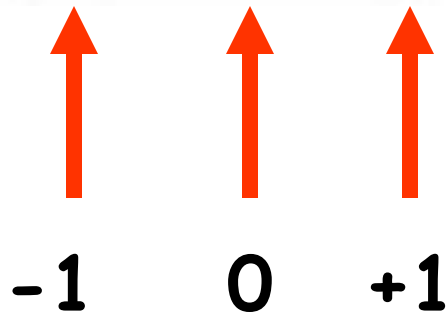
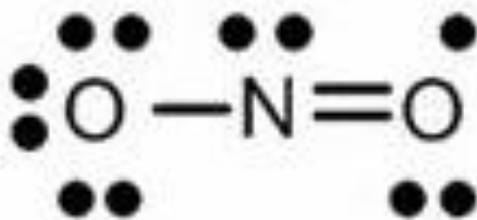
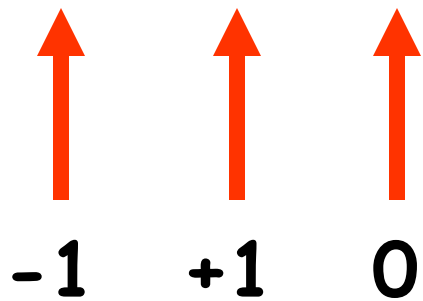
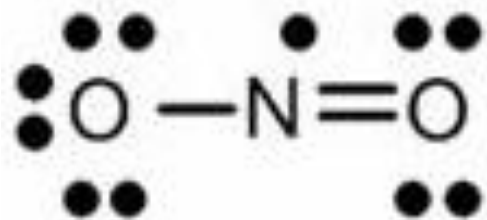
$$(6) - (0) - \frac{1}{2} (12) = 0$$

Sum

$$2 (-1) + (0) + (0) = -2$$

Ex: Nitrogen Dioxide

Use formal charges to decide which is the best resonance structure



Localized Electron Model

Lewis structures are an application of the “Localized Electron Model”

- Electron pairs can be thought of as “belonging” to pairs of atoms when bonding using atomic orbitals. Lone pairs belong to only one atom.

Resonance points out a weakness in LEM!

Other “better” models exist.

- What about Delocalized electrons?

Doesn't work with LEM but we know it happens!

VSEPR Model

Valence Shell Electron Pair Repulsion

- The structure around a given atom is *mostly* determined by minimizing electron pair repulsions.
 - Repulsions minimized by being as far apart from each other as possible. In other words – largest bond angles possible

YOU CAN'T JUST LOOK AT ANGLES BETWEEN THE ATOMS! YOU HAVE TO INCLUDE THE LONE PAIRS TOO! THEY WANT A LOT OF "ELBOW ROOM"

Predicting a VSEPR Structure

- **Draw Lewis structure.**
- **Put pairs as far apart as possible.**
- **Determine positions of atoms from the way electron pairs are shared**
- **Determine the name of molecular structure from positions of the atoms using the AXE formula**

In reality...memorize it all using AXE formulas to help in the memorization process.

VSEPR – AXE Method

- The **A** represents the central atom.
- The **X** represents how many sigma bonds are formed between the central atoms and outside atoms. Multiple covalent bonds (π , double or triple) count as one **X**. Basically, how many atoms are bonded to the central A atom.
- The **E** represents the number of lone electron pairs present on the central atom.
- The sum of **X** and **E** known as the steric number.

VSEPR

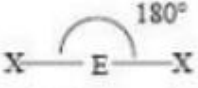
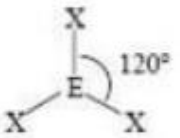
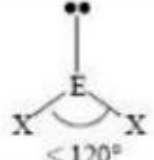
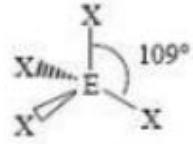
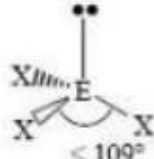

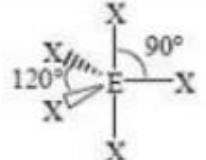
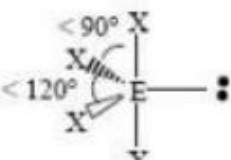
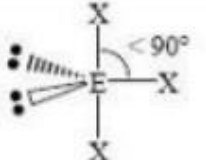
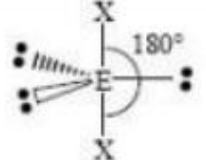
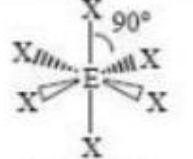
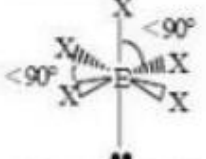
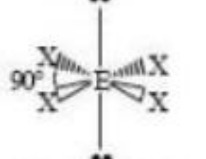
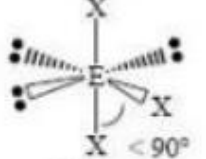
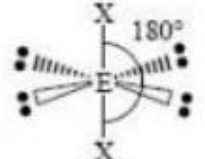
X + E	Overall Structure (Electronic Geometry)	Forms
2	Linear	AX_2
3	Trigonal Planar	AX_3, AX_2E
4	Tetrahedral	AX_4, AX_3E, AX_2E_2
5	Trigonal bipyramidal	$AX_5, AX_4E, AX_3E_2, AX_2E_3$
6	Octahedral	AX_6, AX_5E, AX_4E_2

A = central atom

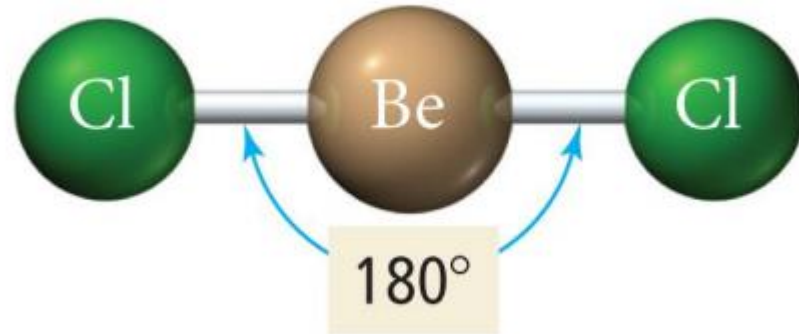
X = atoms bonded to A

E = nonbonding electron pairs on A

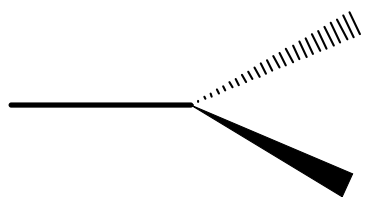
VSEPR

VSEPR Geometries					
Steric No.	Basic Geometry 0 lone pair	1 lone pair	2 lone pairs	3 lone pairs	4 lone pairs
2	 <p>Linear</p>				
3	 <p>Trigonal Planar</p>	 <p>Bent or Angular</p>			
4	 <p>Tetrahedral</p>	 <p>Trigonal Pyramid</p>	 <p>Bent or Angular</p>		
5	 <p>Trigonal Bipyramid</p>	 <p>Sawhorse or Seesaw</p>	 <p>T-shape</p>	 <p>Linear</p>	
6	 <p>Octahedral</p>	 <p>Square Pyramid</p>	 <p>Square Planar</p>	 <p>T-shape</p>	 <p>Linear</p>

AX_2 : Linear (180°)

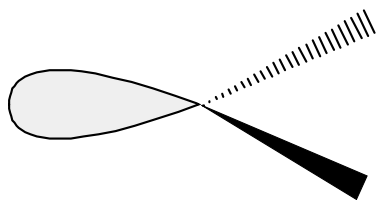


AX_3 , AX_2E : Trigonal Planer (120°)



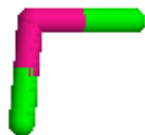
AX_3

BF_3

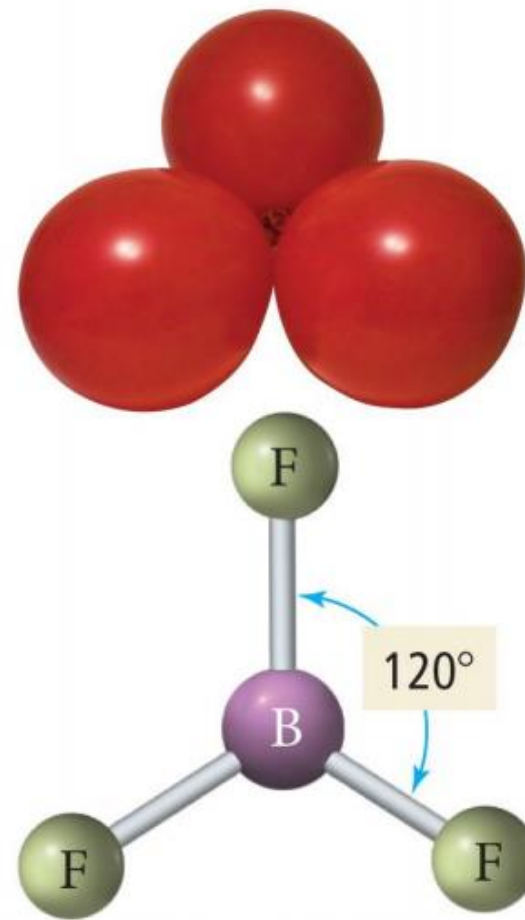


AX_2E
(Bent)

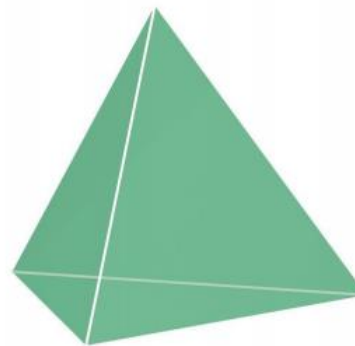
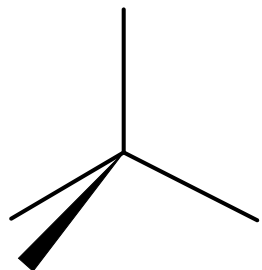
$SnCl_2$



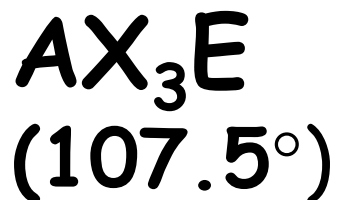
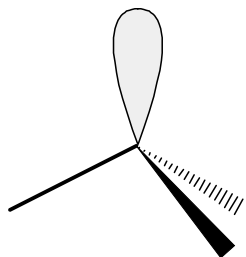
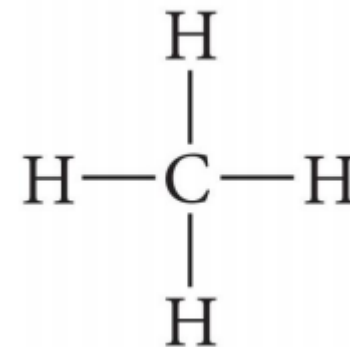
RED = Molecular Geo.



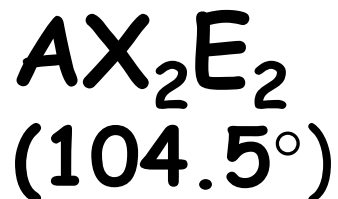
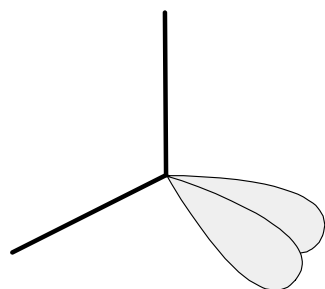
AX_4 , AX_3E , AX_2E_2 : Tetrahedral (109.5°)



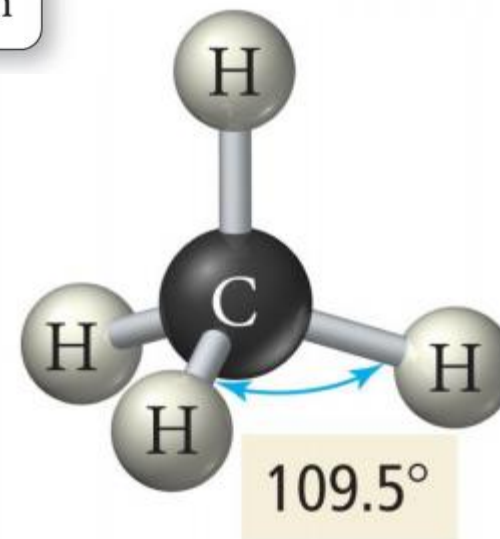
Tetrahedron



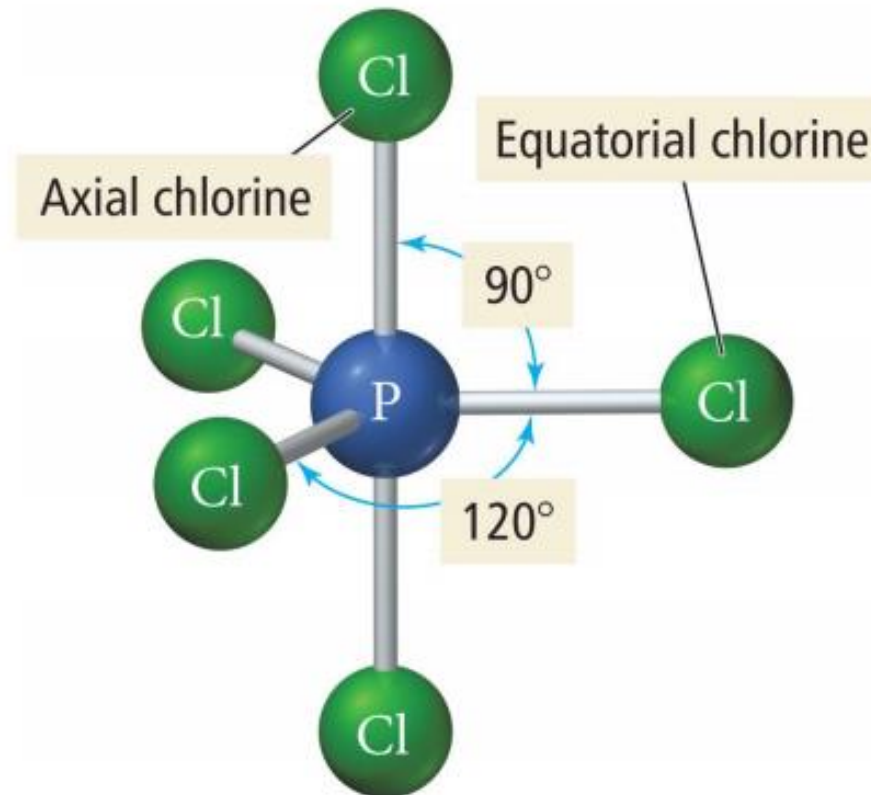
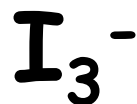
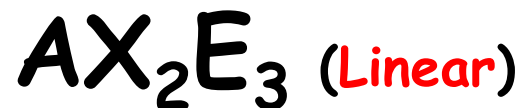
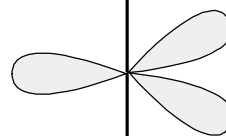
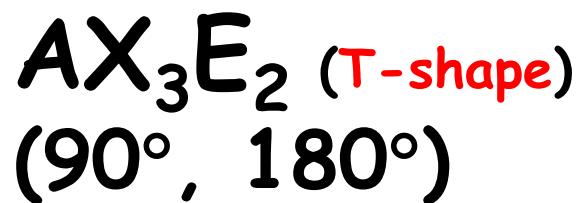
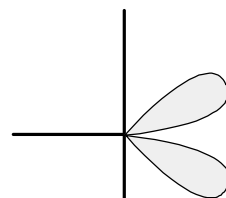
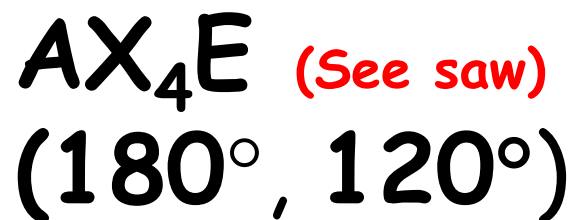
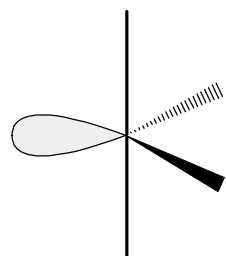
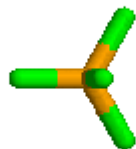
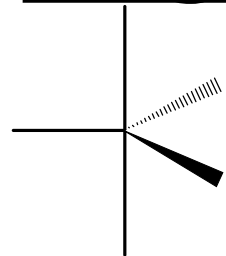
(Trigonal Pyramidal)



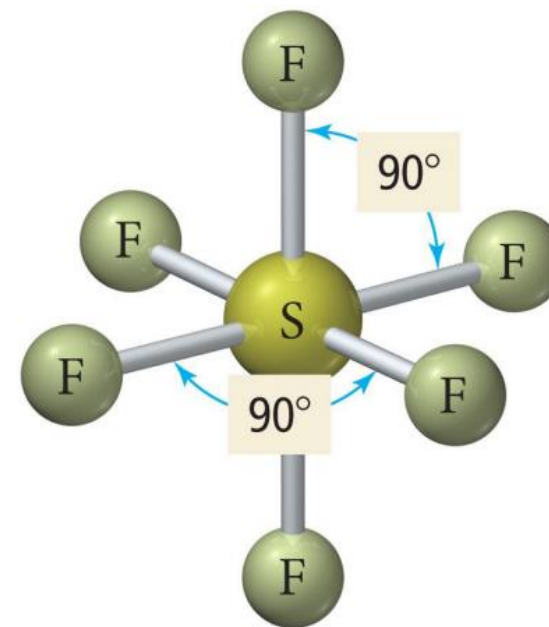
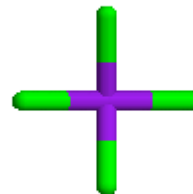
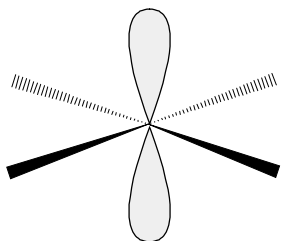
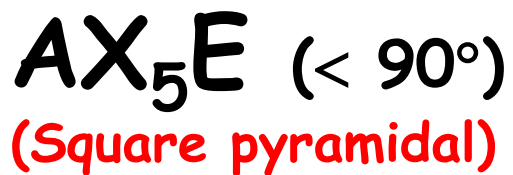
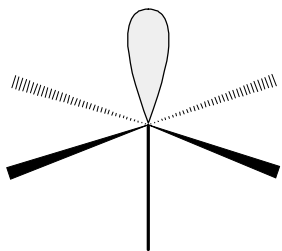
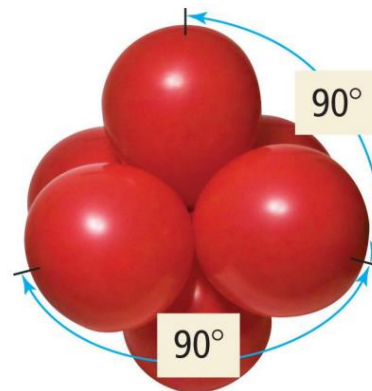
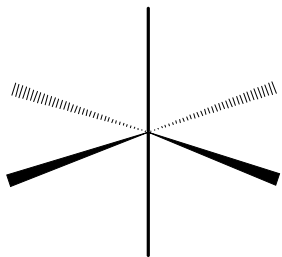
(Bent)



AX_5 , AX_4E , AX_3E_2 , AX_2E_3 : Trigonal Bipyramidal (120° , 90°)

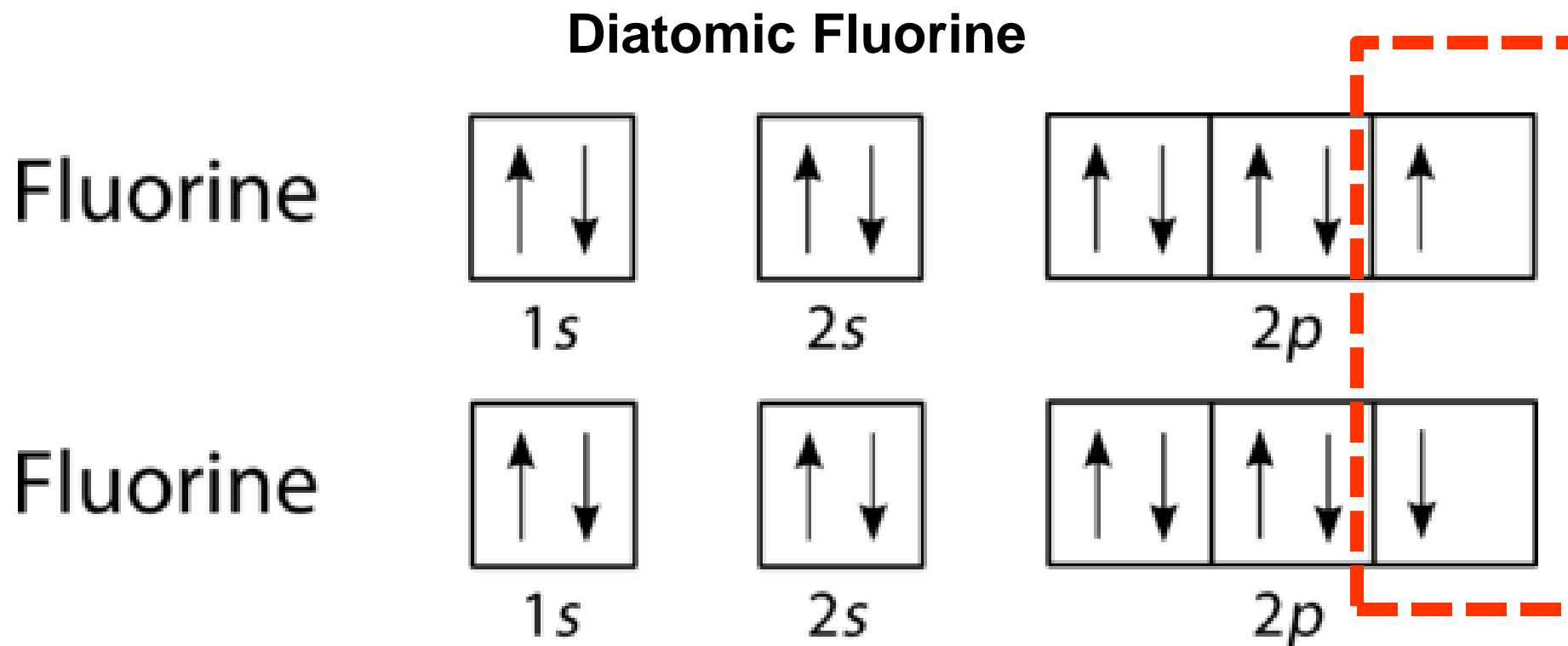


AX_6 , AX_5E , AX_4E_2 : Octahedral (90°)



REMINDER: The Octet Rule

Combinations of elements tend to form so that each atom, by gaining, losing, or sharing electrons, has an octet of electrons in its highest occupied energy level.



Comments About the Octet Rule

2nd period elements

C, N, O, F observe the octet rule

And the H O N C rule as well.

1 2 3 4

of bonds each likes to make

Comments About the Octet Rule

2nd period elements B and Be often have fewer than 8 electrons around themselves - they are very reactive. They have “deficient octets.”

Comments About the Octet Rule

**3rd period elements and beyond
CAN exceed the octet rule to have
expanded octets because those
elements have...d orbitals!
They can have “expanded octets”**

Comments About the Octet Rule

When writing Lewis Structures
satisfy octets first, then if needed place
extra electrons around the central atom.

Comments About the Octet Rule

Don't forget

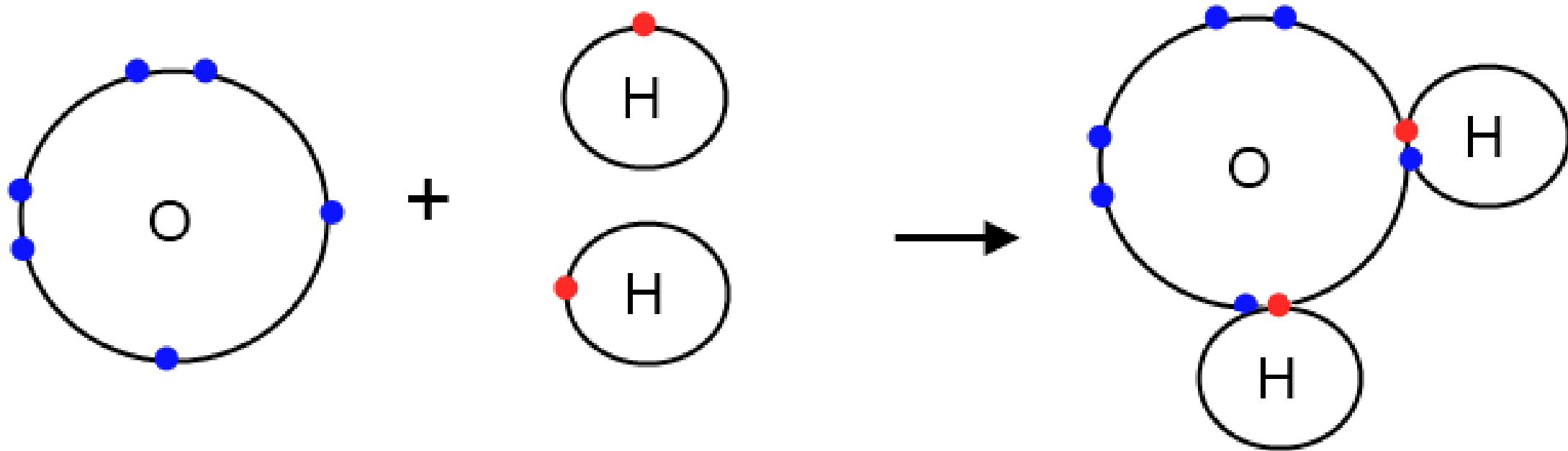
just because an element CAN have an expanded octet (like S) doesn't mean it HAS to. Also, don't forget things like B and Be are fine with a deficient octet – they are fine with fewer electrons.

Comments About the Octet Rule

When writing Lewis Structures

you should technically take into account Formal Charges, but typically a valid structure that follows the octet rule will be accepted unless it says something to allude to needing to take FC into account.

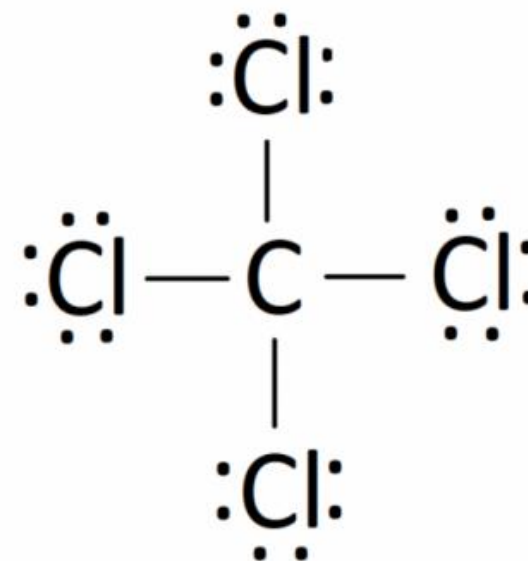
Formation of Water by the Octet Rule



Lewis Structures

- Shows how valence electrons are arranged among atoms in a molecule.
- Reflects central idea that stability of a compound relates to noble gas electron configuration.

Do NOT just randomly throw dots all over your paper! Follow the steps and be thoughtful!



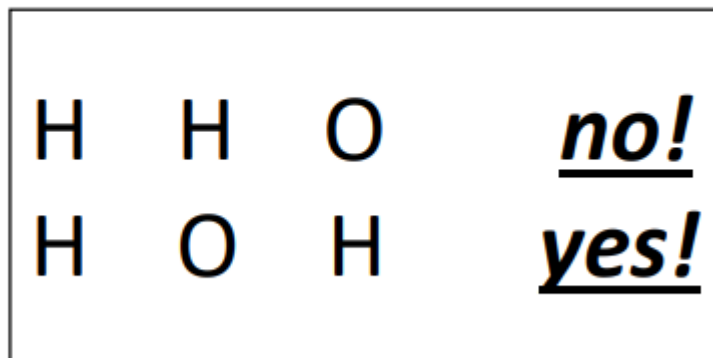
“Rules” for Drawing Lewis Structures

- 1) **Count** and sum valence electrons.
- 2) **Place** your atoms.
- 3) Bond all atoms w/ a **single bond** (try simplest way 1st).
- 4) Give all atoms a **full shell**.
- 5) **Re-count** the electrons you used.
- 6) Used **too few**? Put extras on the central atom.
- 7) Used **too many**? Try double or triple bonds to fix.
- 8) **Re-count**.

Placement Suggestions

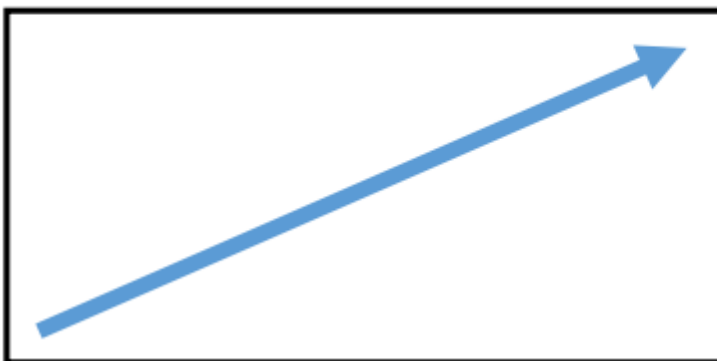
1) Hydrogen always goes on the outside of the molecule

- it is a “dead end”
- it “terminates” the molecule
- it “caps off” the molecule
- Because it can only make 1 bond



2) The least electronegative atom goes in the inside/center

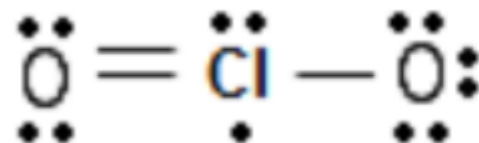
- except for hydrogen!



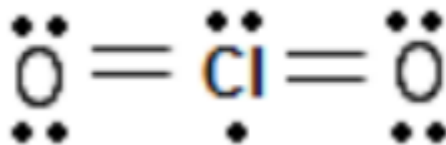
Placement Suggestions

3) Symmetry is good!

- When possible!



Fine but not great



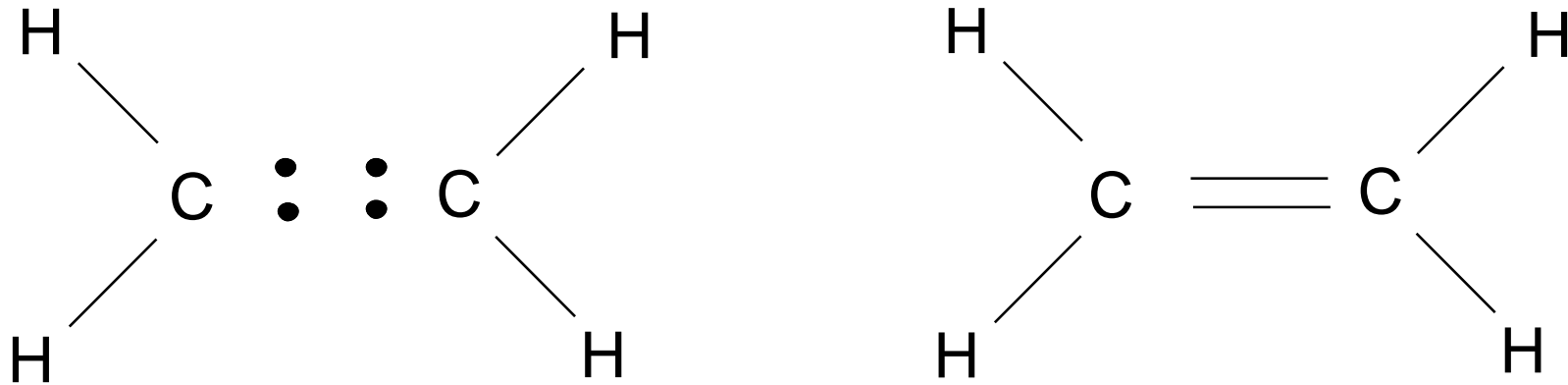
Better! Symmetrical!

4) Think about Formal Charges

- Want lowest formal charges
- If drawing an ion, sum of formal charges should match the charge on the ions
- Negative FC on more electronegative elements

Multiple Covalent Bonds:

Double bonds

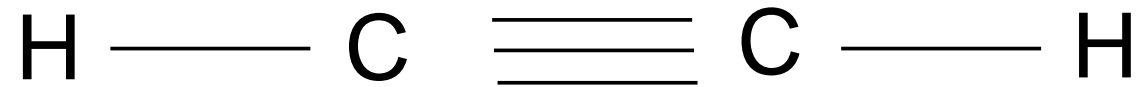
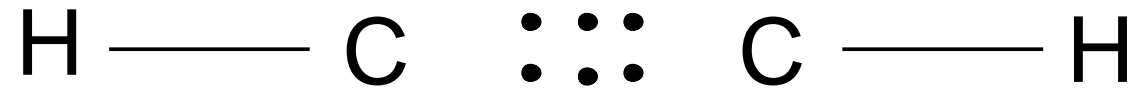


Ethene

Two pairs of shared electrons

Multiple Covalent Bonds:

Triple bonds



Ethyne

Three pairs of shared electrons