N21 – Bonding

Formal Charge and VSEPR

Link to YouTube Presentation: https://youtu.be/KvJ2DPLVjfI

N21 – Bonding

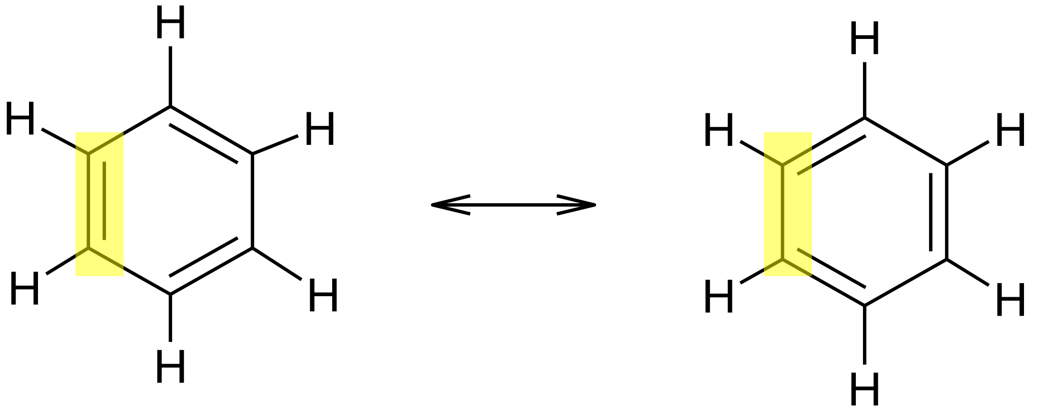
Formal Charge and VSEPR

Target: I can draw more accurate and preferred Lewis Structures by considering Resonance Structures, Formal Charge, and VSEPR Theory

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.

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.

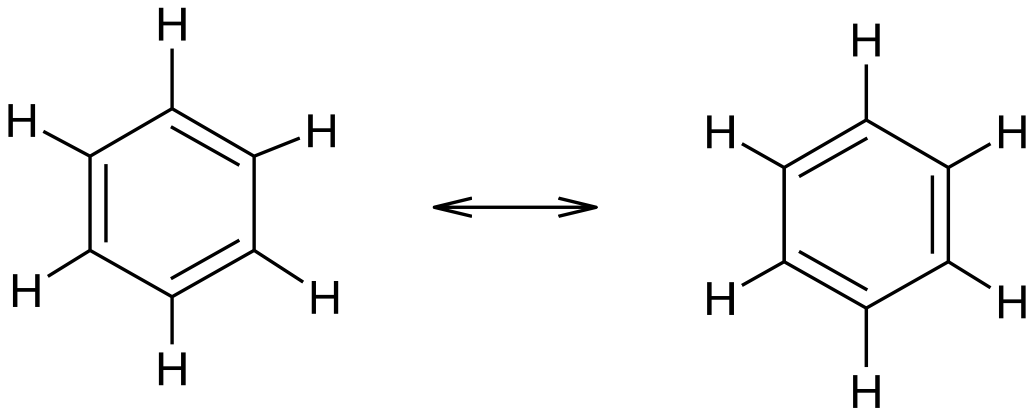
Resonance points out a weakness in LEM!
Other "better" models exist.

- What about Delocalized electrons?
  Doesn't work with LEM but we know it happens!

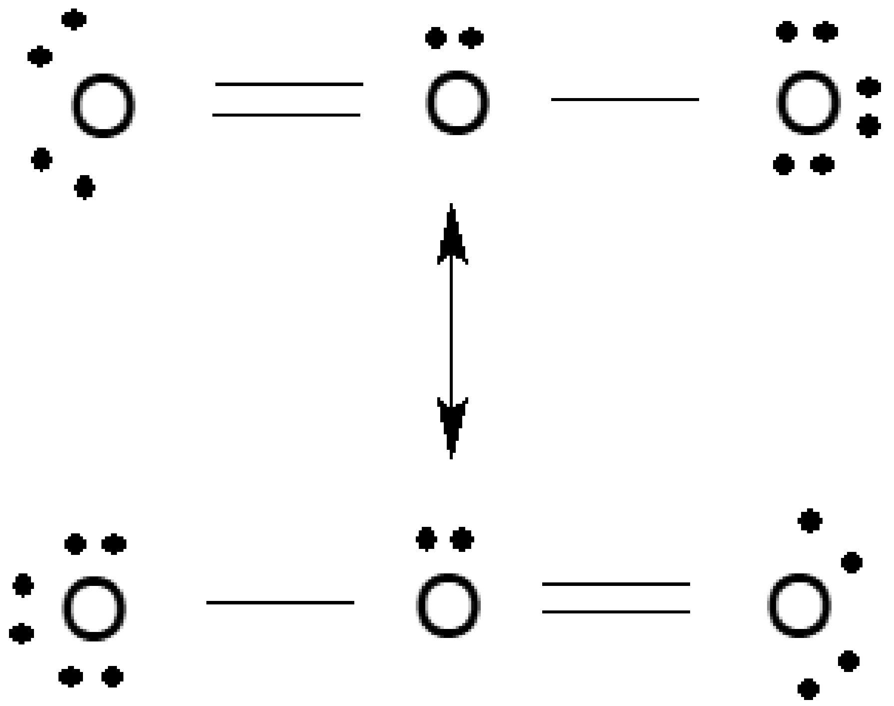
Resonance Bond Length and Energy

Resonance bonds are **shorter**
and **stronger** than single bonds.

Resonance bonds are **longer**
and **weaker** than double bonds.



Resonance in Ozone, O_3



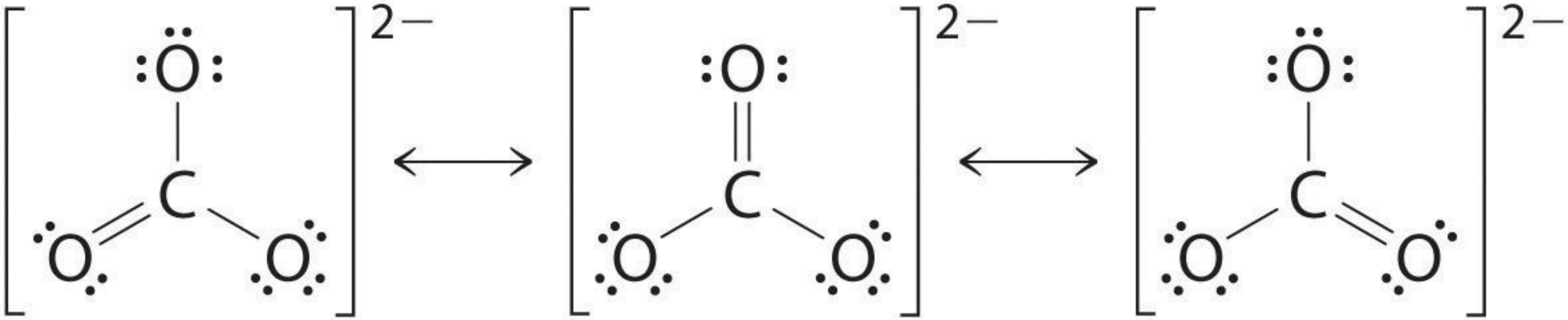
Neither structure is correct!

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

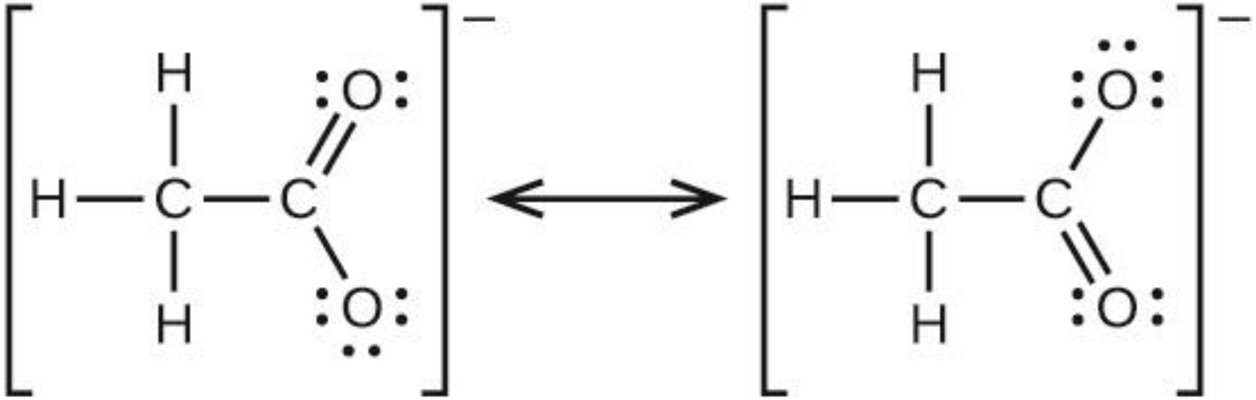
We know this from experimental data!

Resonance in Polyatomic Ions

Resonance in a carbonate ion:



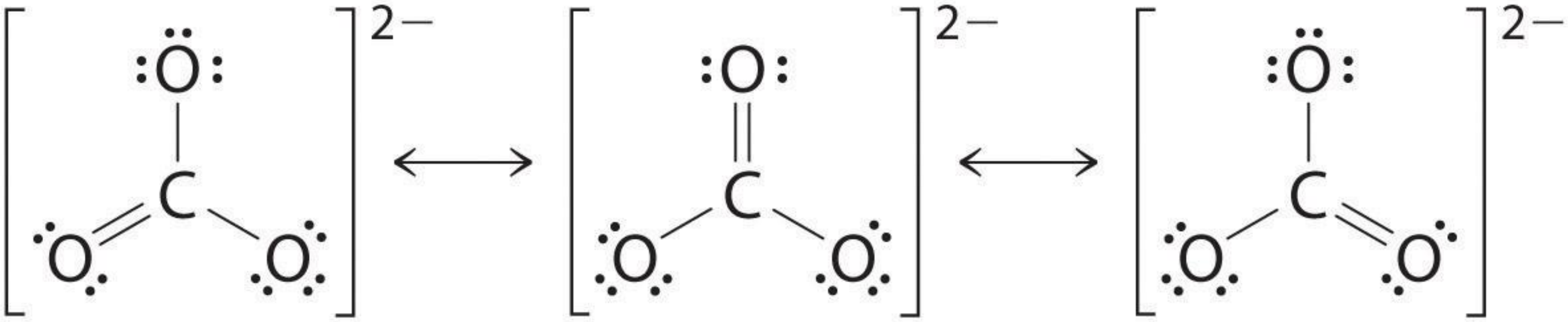
Resonance in an acetate ion:



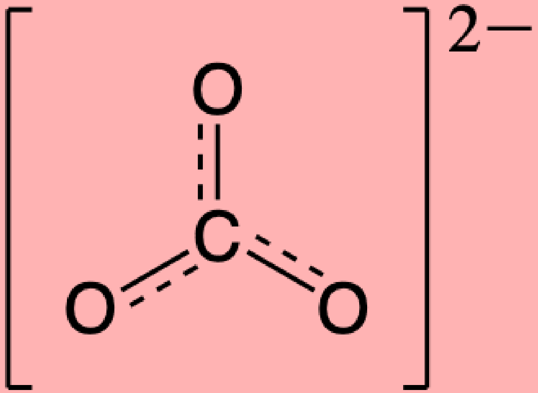
Use square brackets and double headed arrows between resonance structures!

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.



CAREFUL! **DO NOT DO THIS IF THEY ASK YOU TO DRAW THE RESONANCE STRUCTURES!**
NO POINTS FOR ONE STRUCTURE WITH DOTTED LINES!

Formal Charge

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

Formal Charge helps us figure out which is best
“The charge assigned to an atom in a molecule, assuming that the electrons in all chemical bonds are shared equally between atoms, regardless of relative electronegativities.”

Basically –
what charge would the atoms have if you divvied up the electrons equally and they were all separate atoms again.

How to Calculate Formal Charge

Formal Charge = Should - Has

# of Valence e- - (# lone pair e^-'s on the atom + ½ the # of bonded e-)

From the periodic table!

Half because they are sharing with the other atom

How to Calculate Formal Charge

Formal Charge = Should - Has

# of Valence e- - (# lone pair e^-’s on the atom + ½ the # of bonded e-)

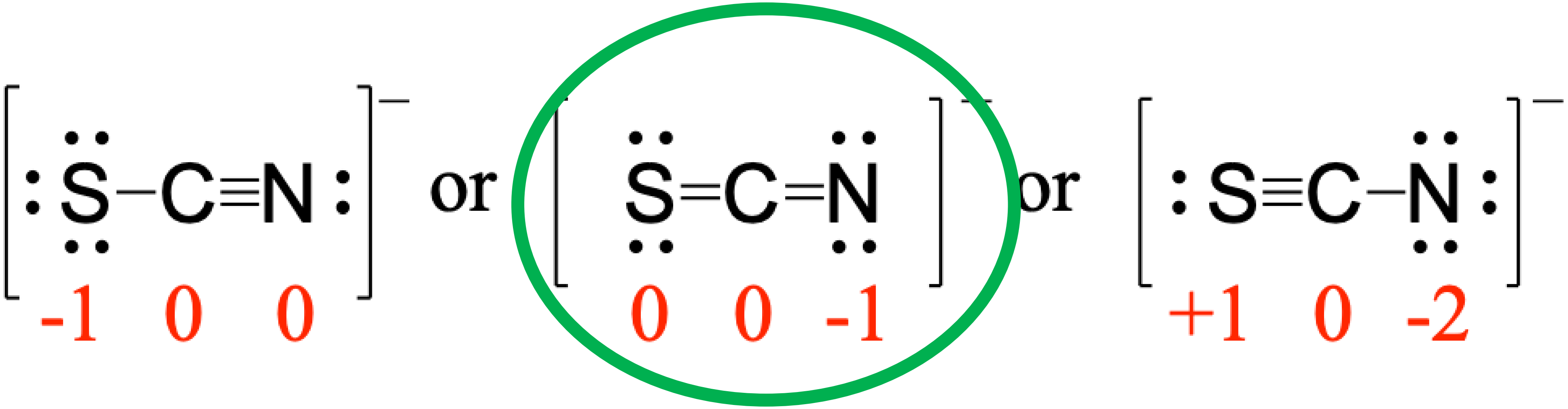
Half because they are sharing with the other atom

Formal Charge

Which structure is preferred?

- Minimizing the “formal charge” on the atoms,

  AND
- Having negative Formal Charge on the more electronegative elements



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.

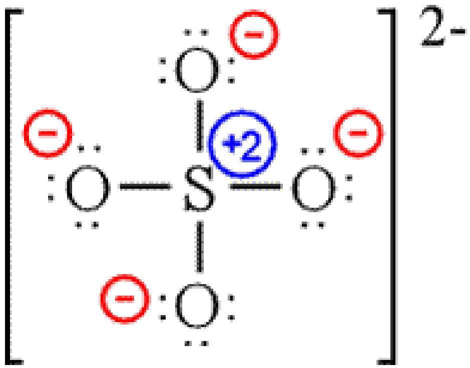
AND

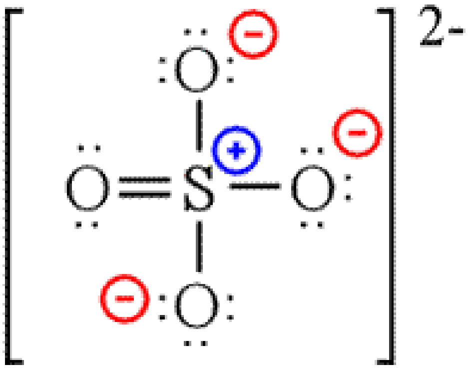
- The sum of all FC must equal the overall charge on the ion or molecule.

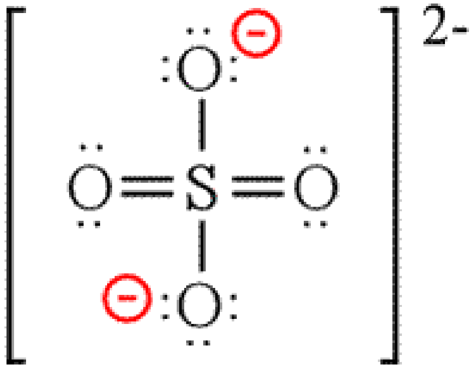
- this is the one people forget about!

Ex: Sulfate Ion

FC = # of Valence e- - # lone pair e^-'s on the atom - ½ the # of bonded e-







Each Oxygen:
(6) – (6) – ½ (2) = -1

Sulfur:
(6) – (0) – ½ (8) = +2

Sum
4 (-1) + (+2) = -2
Good, that matches the charge on the sulfate ion!

Single Bonded Oxygens
(6) – (6) – ½ (2) = -1

Double Bonded Oxygen:
(6) – (4) – ½ (4) = 0

Sulfur:
(6) – (0) – ½ (10) = +1

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

Single Bonded Oxygen:
(6) – (6) – ½ (2) = -1

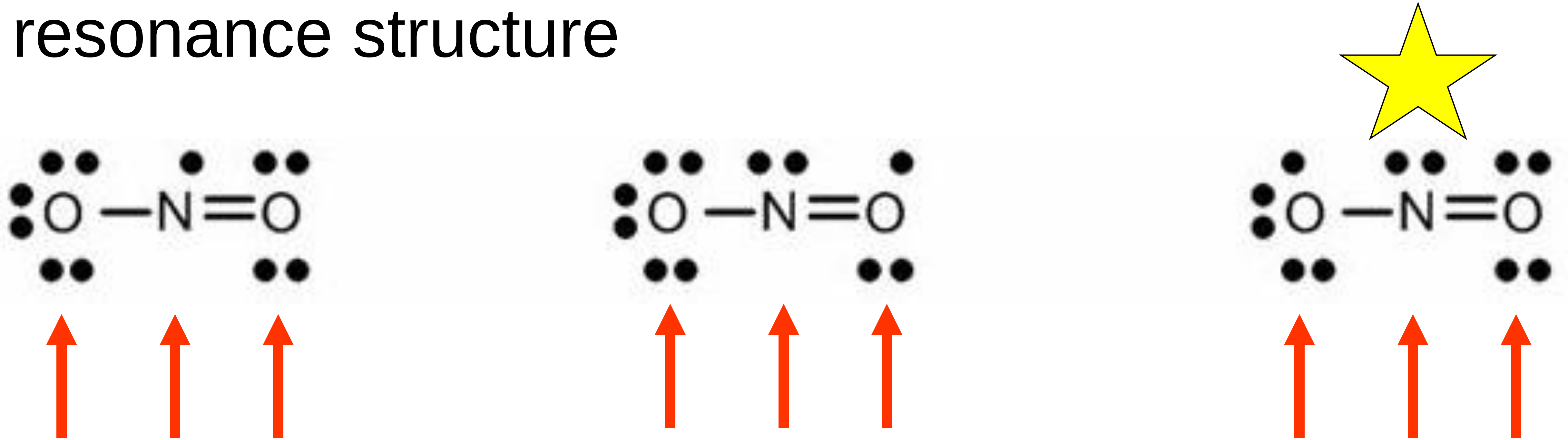
Double Bonded Oxygens:
(6) – (4) – ½ (4) = 0

Sulfur:
(6) – (0) – ½ (12) = 0

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

Ex: Nitrogen Dioxide

Use formal charges to decide which is the best resonance structure



-1 +1 0

-1 0 +1

0 0 0

Rest of this PowerPoint is review of VSEPR and Lewis Structures.

If you need a refresher then keep going, or even go watch the Honors Chem lecture videos on these topics!

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

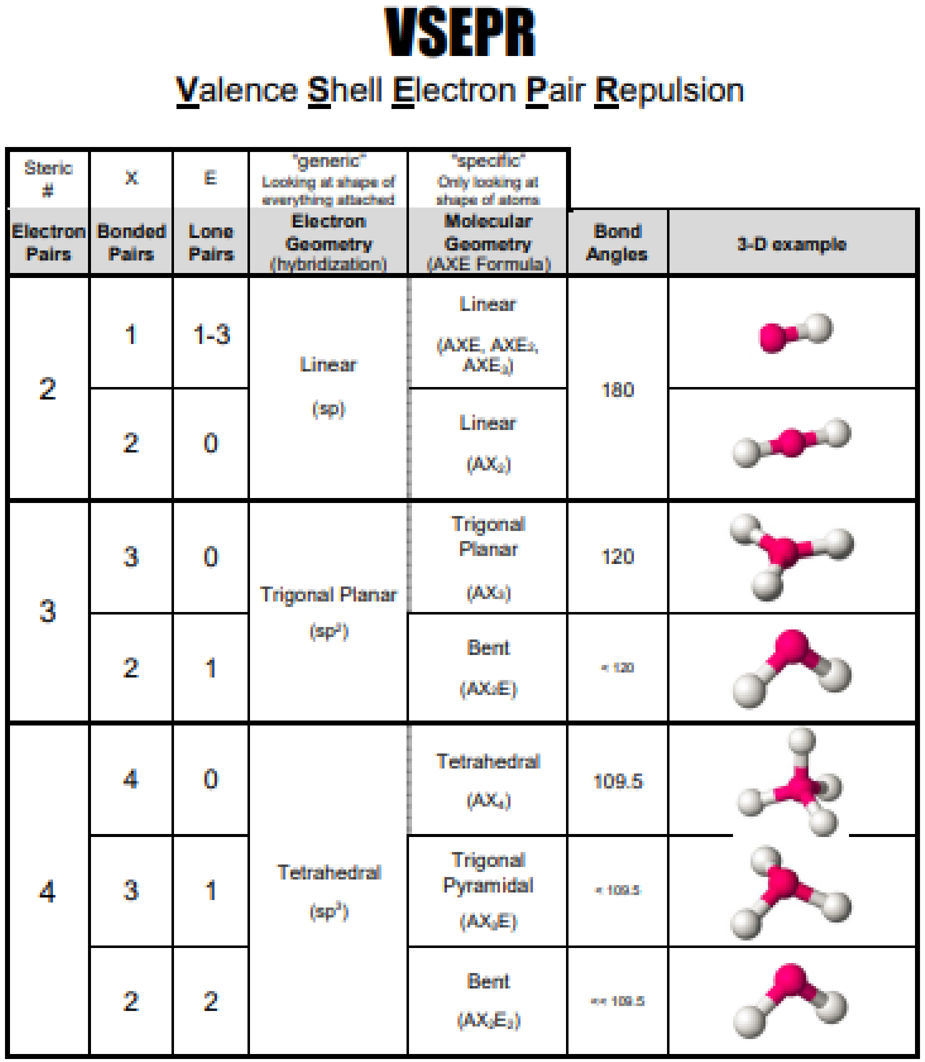
X + E	Overall Structure (Electronic Geometry)	Forms
2	Linear	AX_2
3	Trigonal Planar	AX_3, AX_2E
4	Tetrahedral	AX_4, AX_3E, AX_2E_2
5	Trigonal bipyramidal	AX_5, AX_4E, AX_3E_2, AX_2E_3
6	Octahedral	AX_6, AX_5E, AX_4E_2

A = central atom

X = atoms bonded to A

E = nonbonding electron pairs on A

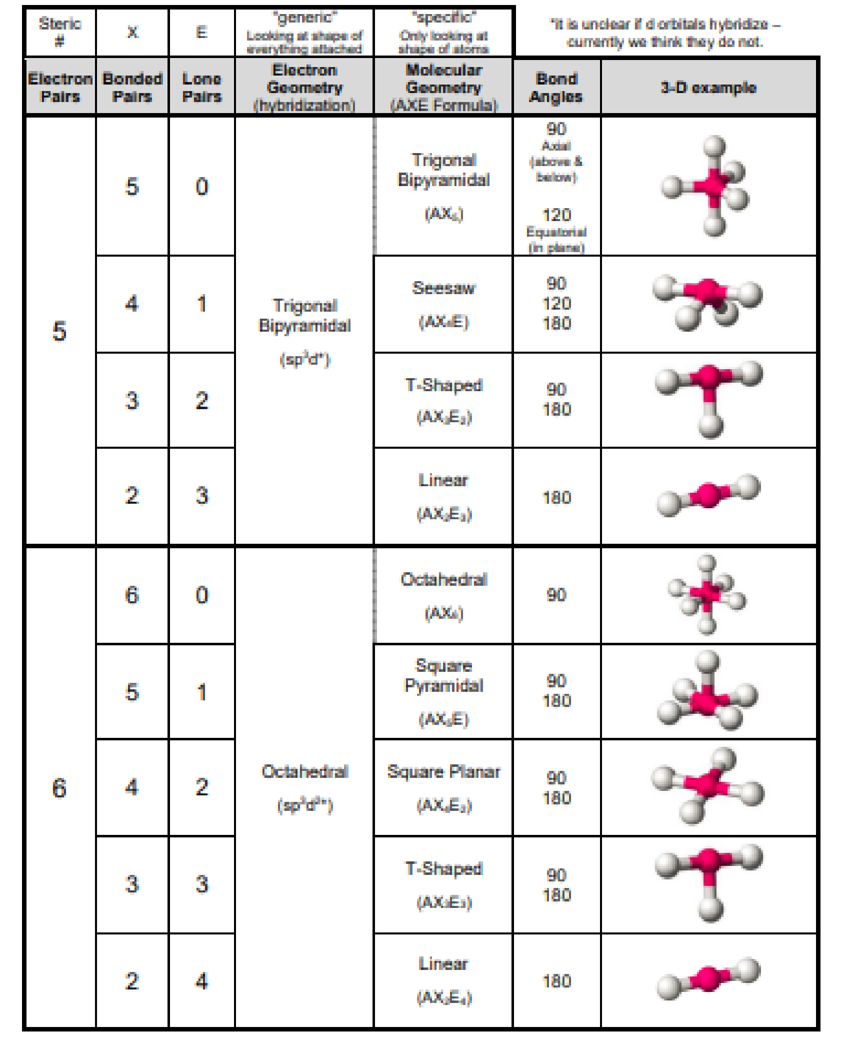
VSEPR



VSEPR

Valence Shell Electron Pair Repulsion

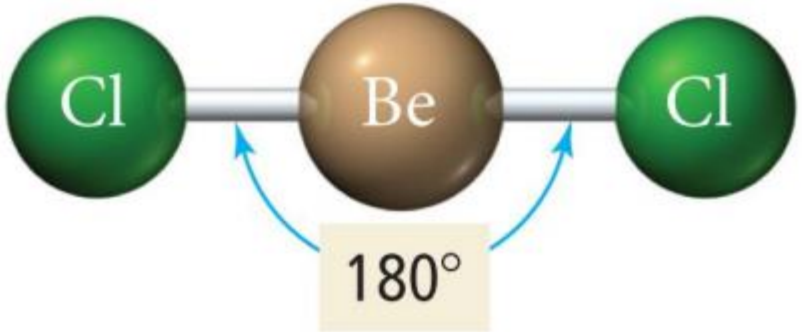
Steric #	X	E	"generic" Looking at shape of everything attached	"specific" Only looking at shape of atoms		
Electron Pairs	**Bonded Pairs**	**Lone Pairs**	**Electron Geometry** (hybridization)	**Molecular Geometry** (AXE Formula)	**Bond Angles**	**3-D example**
2	1	1-3	Linear (sp)	Linear (AXE, AXE_2, AXE_3)	180	
	2	0		Linear (AX_2)		
3	3	0	Trigonal Planar (sp^2)	Trigonal Planar (AX_3)	120	
	2	1		Bent (AX_2E)	< 120	
4	4	0	Tetrahedral (sp^3)	Tetrahedral (AX_4)	109.5	
	3	1		Trigonal Pyramidal (AX_3E)	< 109.5	
	2	2		Bent (AX_2E_2)	<< 109.5	



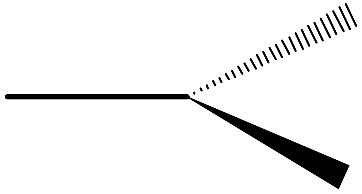
Steric #	X	E	"generic" Looking at shape of everything attached	"specific" Only looking at shape of atoms		
Electron Pairs	**Bonded Pairs**	**Lone Pairs**	**Electron Geometry** (hybridization)	**Molecular Geometry** (AXE Formula)	**Bond Angles**	**3-D example**
5	5	0	Trigonal Bipyramidal (sp^3d^*)	Trigonal Bipyramidal (AX_5)	90 Axial (above & below) 120 Equatorial (in plane)	
	4	1		Seesaw (AX_4E)	90 120 180	
	3	2		T-Shaped (AX_3E_2)	90 180	
	2	3		Linear (AX_2E_3)	180	
6	6	0	Octahedral (sp^3d^{2*})	Octahedral (AX_6)	90	
	5	1		Square Pyramidal (AX_5E)	90 180	
	4	2		Square Planar (AX_4E_2)	90 180	
	3	3		T-Shaped (AX_3E_3)	90 180	
	2	4		Linear (AX_2E_4)	180	

*it is unclear if d orbitals hybridize – currently we think they do not.

AX_2: Linear (180°)

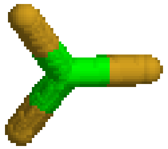


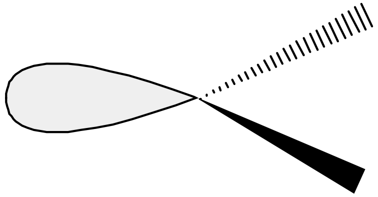
AX$_3$, AX$_2$E: Trigonal Planer (120°)



AX$_3$

BF$_3$

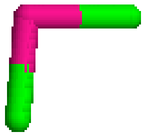


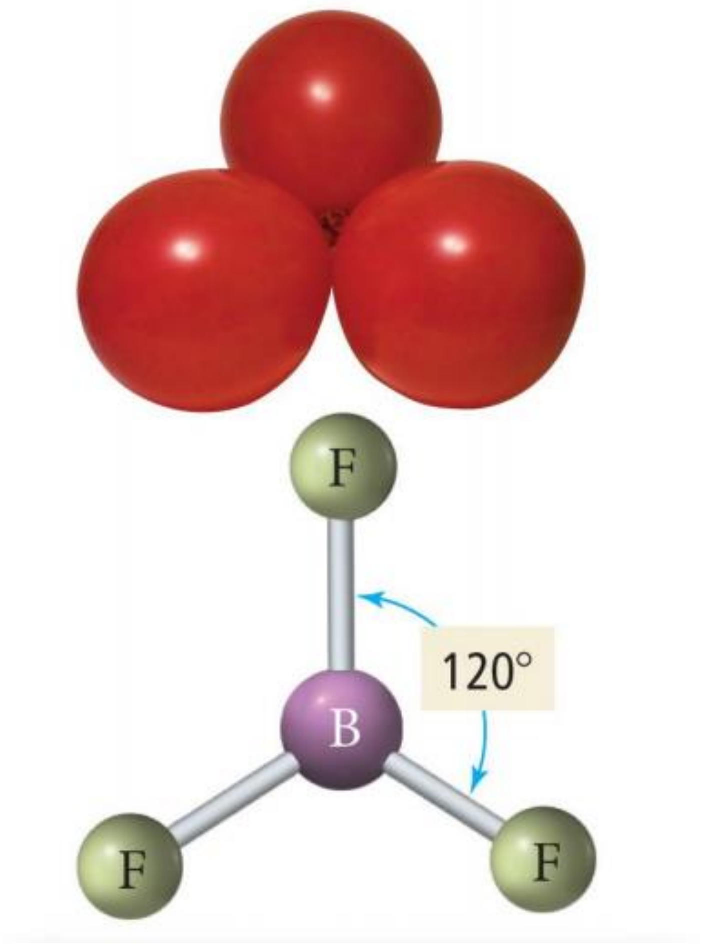


AX$_2$E

(Bent)

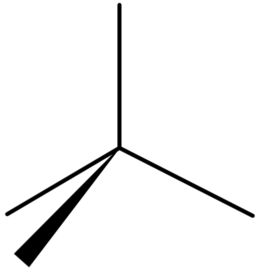
SnCl$_2$



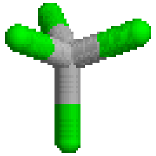


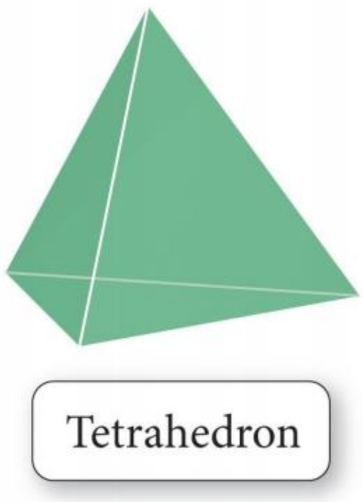
RED = Molecular Geo.

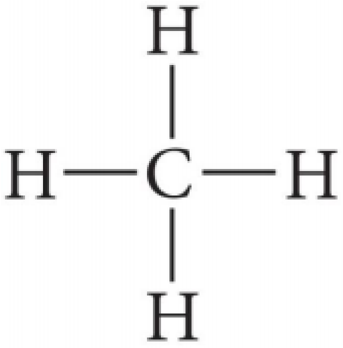
AX_4, AX_3E, AX_2E_2: Tetrahedral (109.5°)

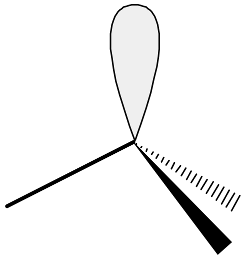


AX_4 CCl_4





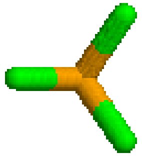


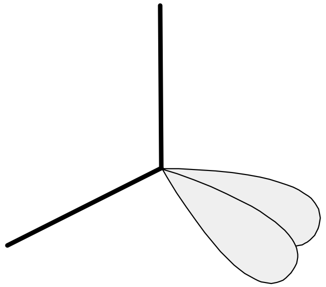


AX_3E PCl_3

(107.5°)

(Trigonal Pyramidal)

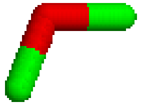


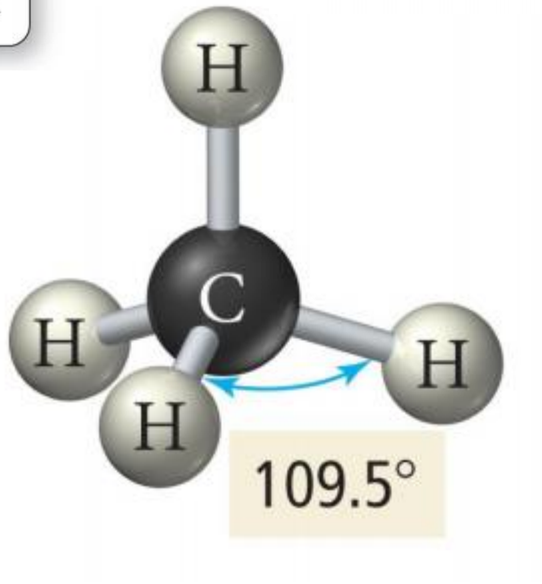


AX_2E_2 Cl_2O

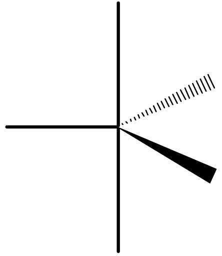
(104.5°)

(Bent)

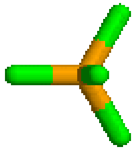


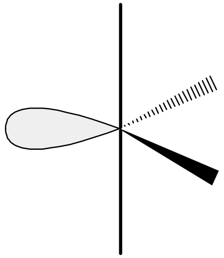


AX_5, AX_4E, AX_3E_2, AX_2E_3 :
Trigonal Bipyramidal (120°, 90 °)

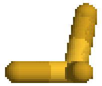


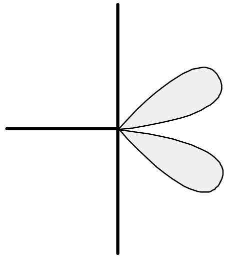
AX_5 PCl_5



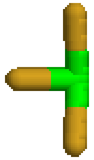


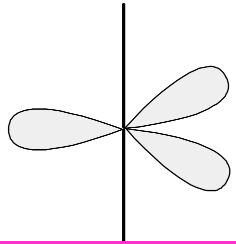
AX_4E (See saw)
(180°, 120°) SF_4



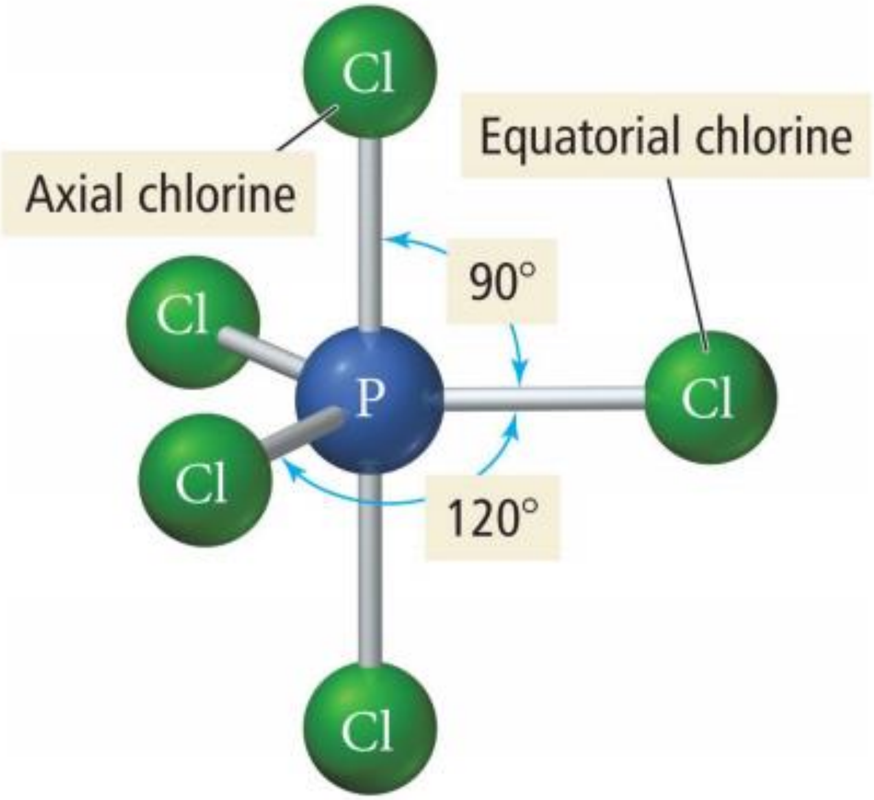


AX_3E_2 (T-shape)
(90°, 180°) ClF_3

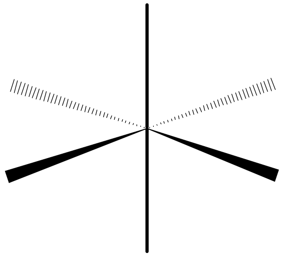




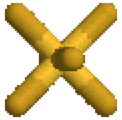
AX_2E_3 (Linear) I_3^-

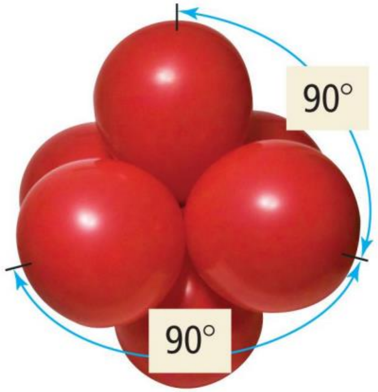


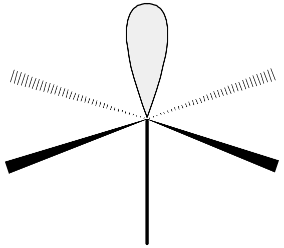
AX_6, AX_5E, AX_4E_2: Octahedral (90°)



AX_6 SF_6

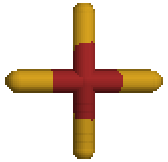


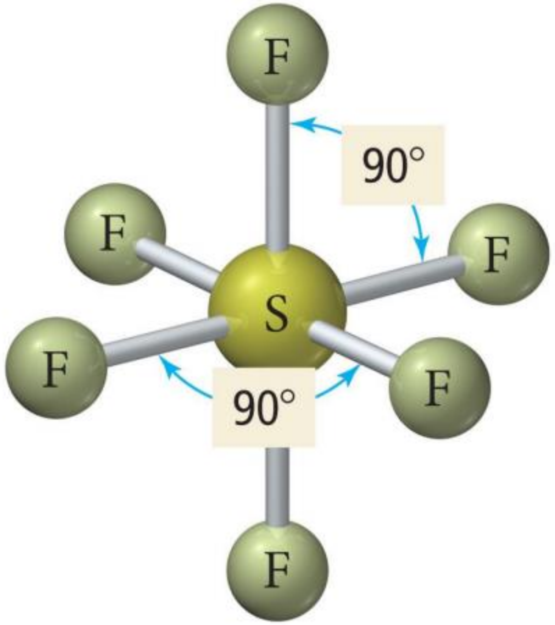


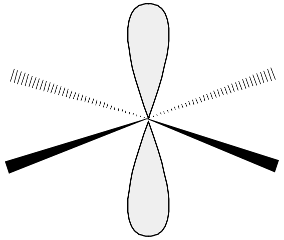


AX_5E (< 90°) BrF_5

(Square pyramidal)

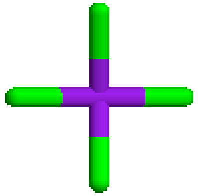






AX_4E_2 (90°) ICl_4-

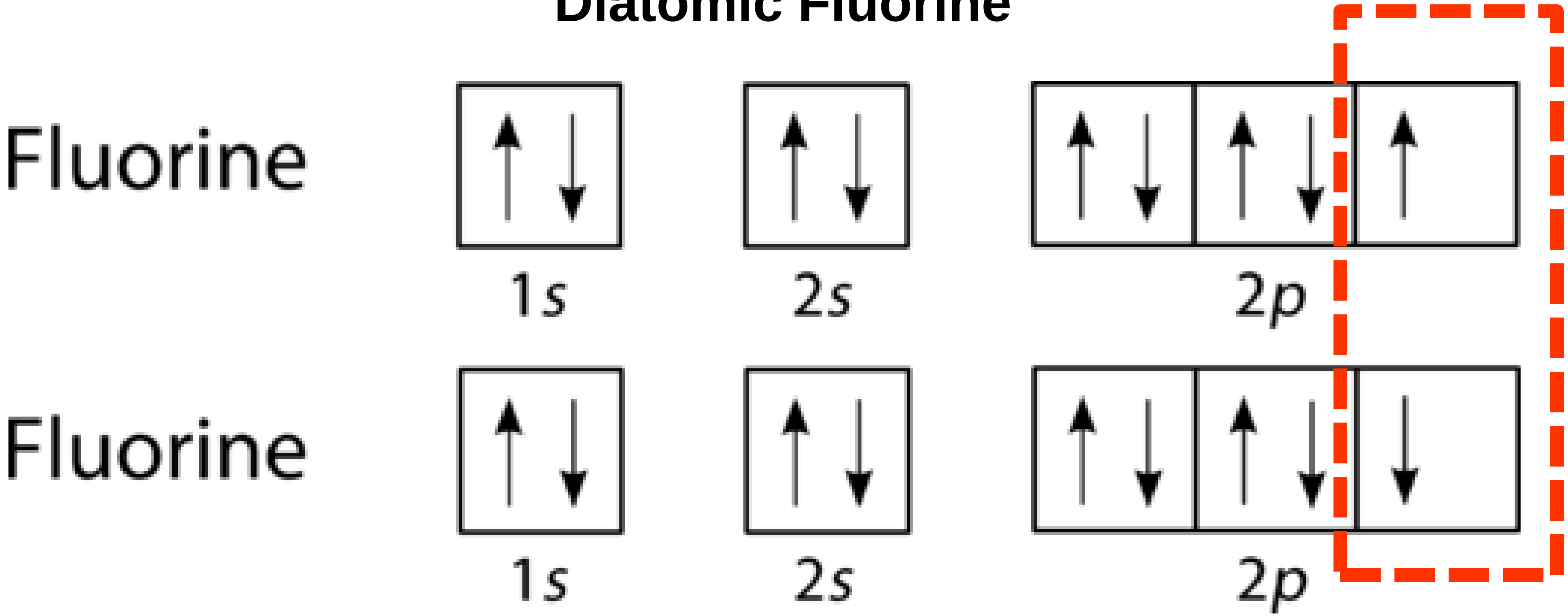
(Square Planar)



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.

Diatomic Fluorine



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 access to…d orbitals! They can have “expanded octets”

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.

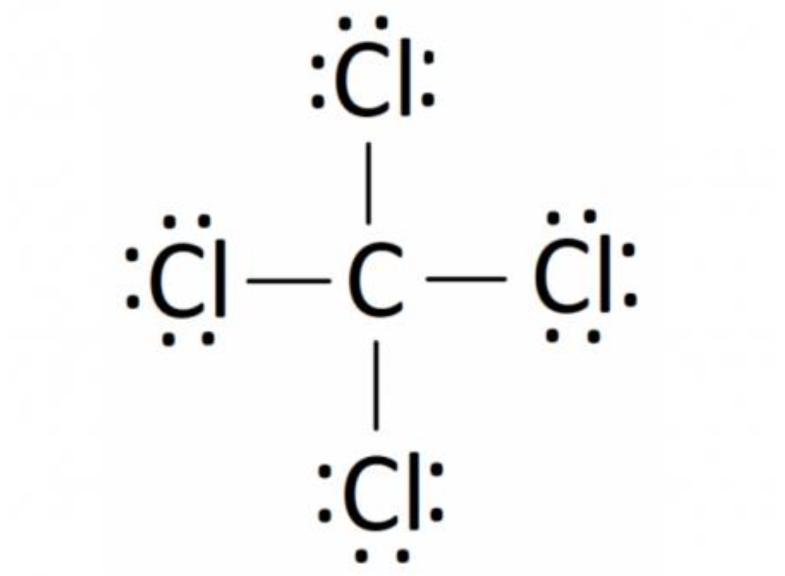
Comments About the Octet Rule

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.

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) Fix if needed
    - Used **too few**? Put extras on the central atom.
    - Used **too many**? Try double or triple bonds to fix.

Placement Suggestions

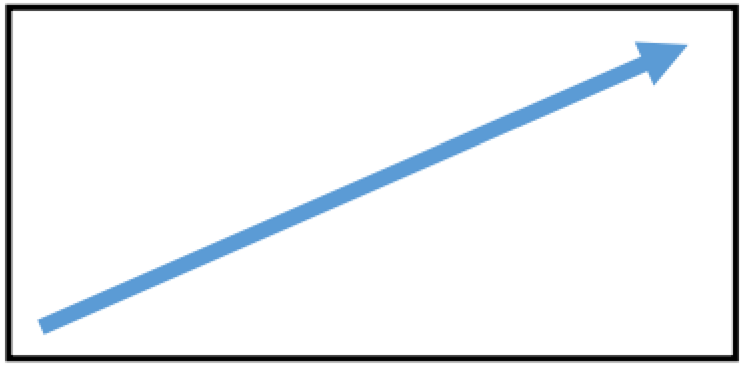
1) **Hydrogen *always* goes on the outside of the molecule**

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

H H O ***no!***
H O H ***yes!***

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

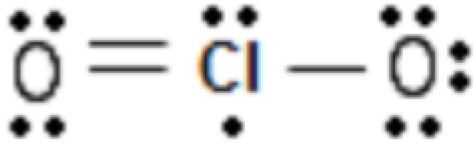
- except for hydrogen!



Placement Suggestions

3) Symmetry is good!

- When possible!



Fine but not great

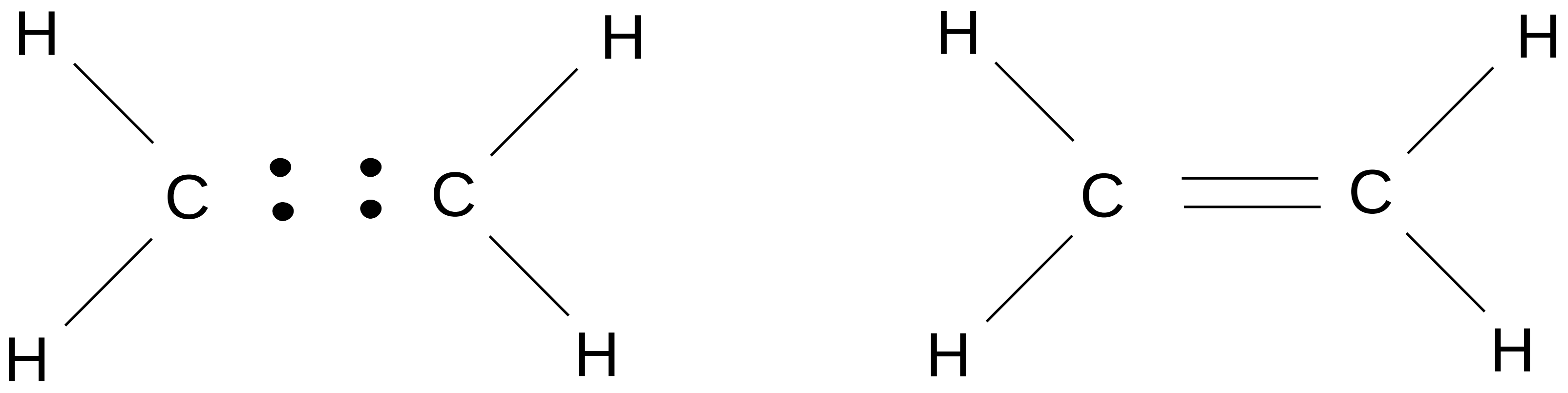
Better! Symmetrical!

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

FOUR electrons being shared

Multiple Covalent Bonds:

Triple bonds

$$\mathrm{H - C :: : C - H}$$

$$\mathrm{H - C \equiv C - H}$$

Ethyne

Three pairs of shared electrons

SIX electrons being shared

YouTube Link to Presentation:

https://youtu.be/KvJ2DPLVjfI