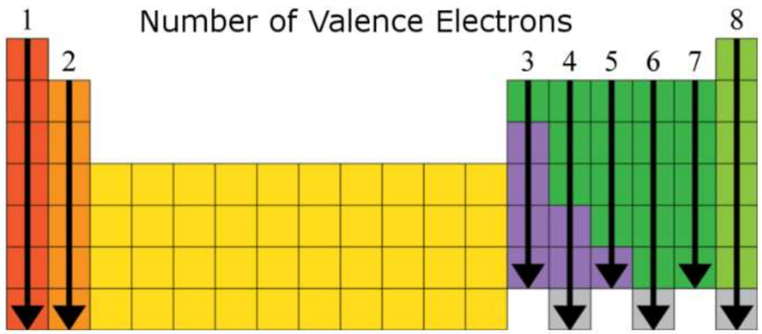
Add up valence electrons for all atoms
Cations – lose electrons: <u>subtract</u> the charge
Anion – gain electrons: <u>add</u> the charge



Calculate Number of Valence Electrons

Ex: NH_4^+

N = 5
4 (H) = 4(1)
Charge = -1

Valence e^- = 8

Ex: CO_3^{-2}

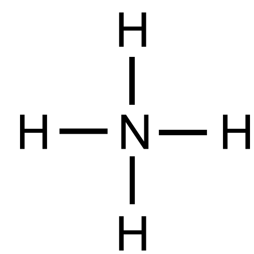
C = 4
3 (O) = 3(6)
Charge = +2

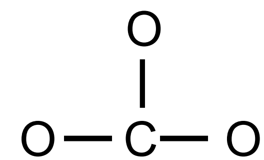
Valence e^- = 24

Build a Trial Structure Using the Following Guidelines

1. Place the least EN element in the middle
2. Arrange other atoms around it to make molecules as symmetrical as possible
3. Draw one bond connecting atoms together
4. H makes 1 bond (never in middle)
5. F, Cl, Br, I form 1 bond (in CHE 101) (never in the middle)
6. Oxygen never bonds to oxygen (in CHE 101)
7. Typical Bonding Patterns – H=1, O = 1 or 2, C =4, N = 1,2,3 and rarely 4 (if it is part of a polyatomic ion).

Build a Trial Structure





Count the electrons left after making your trial structure

Remaining e^- = Valence e^- - 2 (# of Bonds)

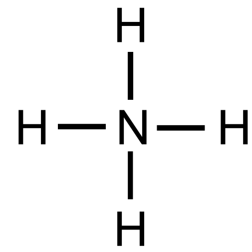
Count Electron Left

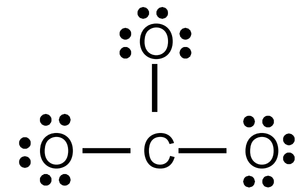
	NH_4^+		CO_3^{-2}
Valence e^- :	8	Valence e^- :	24
- 2 (# of Bonds):	– 2·(4)	- 2 (# of Bonds):	– 2·(3)
Remaining e^-:	0	Remaining e^-:	18

Distribute electrons to complete octets
(noble gas configurations)

1. After you have made your trial structure, start to complete octets until you run out of electrons.
2. Start with the most EN element first.
3. Remember H has an "octet" with 2 electrons

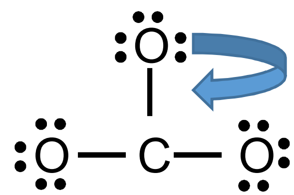
Distribute Electrons





Complete Octets

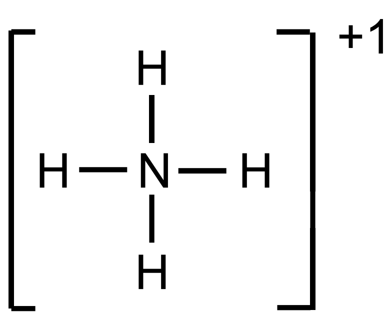
If some atoms can't complete octets remove unshared electron pairs and form double or triple bonds.



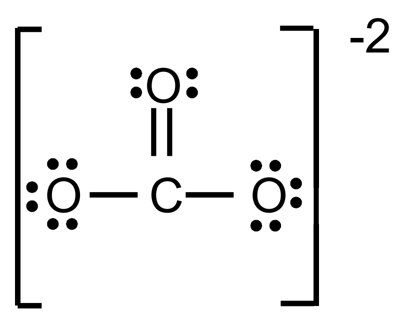
Share the lone pair of electrons on oxygen with the carbon to complete carbons octet.

If all atoms have complete octets = Done!

Remember to put cations/anions in brackets and include the charge



Remember to put cations/anions in brackets and include the charge

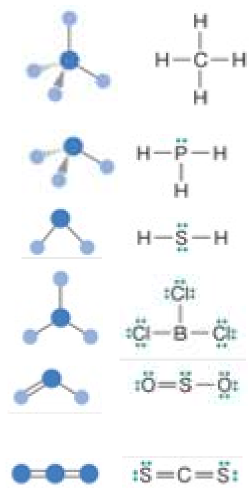


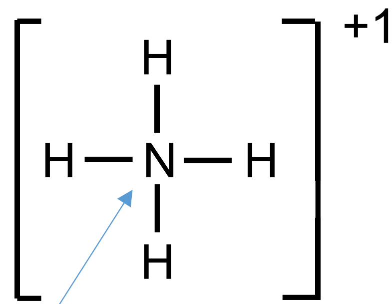
Determine the Shape and Bond Angle

Valence Shell Electron Pair Repulsion Theory (VSEPR)

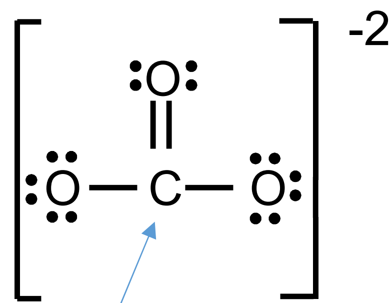
VSEPR Theory predicts the shapes of molecules by realizing that electrons will repulse each other and seek to stay as far apart as possible. It depends on the number of atoms bonded and the number of lone pairs around the central atom. This leading to the following idealized molecular shapes:

# atoms Bonded	# lone pairs	Shape	Bond Angle
4	0	Tetrahedral	109.5
3	1	Trigonal Pyramidal	109.5
2	2	Bent - 109.5	109.5
3	0	Trigonal Planar	120
2	1	Bent - 120	120
2	0	Linear	180





4 atoms, 0 lone pair
Tetrahedral – 109.5

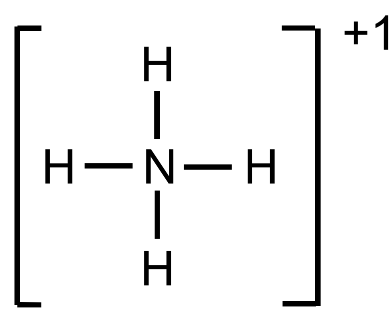


3 atoms, 0 lone pair
Trigonal Planar – 120

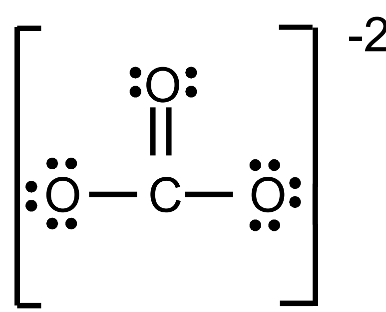
Polarity
Nonpolar or Dipolar

Nonpolar – symmetrical distribution of electron density around a molecule.

Dipolar – unsymmetrical distribution of electron density around a molecule. Molecule will behave like a magnet.



Symmetrical therefore Nonpolar



Symmetrical therefore Nonpolar

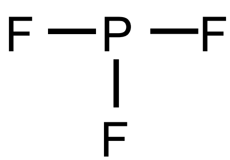
A few more examples…

Phosphorus Trifluoride (PF_3)

1. Count Valence Electron

P = 5
3 (F) = 3(7)
Valence e^- = 26

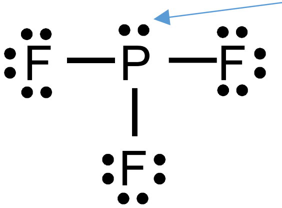
2. Trial Structure



3. Remaining Electrons

Valence e^- :	26
- 2 (# of Bonds):	– 2·(3)
Remaining e^-:	20

4. Complete Octets



3 atoms, 1 lone pair
Trigonal Pyramidal – 109.5

Unsymmetrical Molecule
Therefore Dipolar

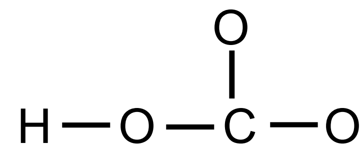
5. Shapes
6. Polarity

Bicarbonate Anion (HCO_3^{-1})

1. Count Valence Electron

H = 1
C = 4
3 (O) = 3(6)
Anion (add) = 1
Valence e^- = 24

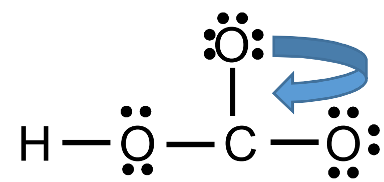
2. Trial Structure



3. Remaining Electrons

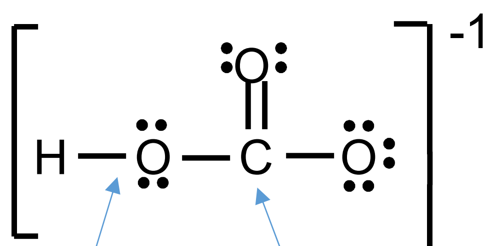
Valence e^- :	24
- 2 (# of Bonds):	– 2·(4)
Remaining e^-:	16

4. Complete Octets/Share e^-



Share the lone pair of electrons on oxygen with the carbon to complete carbons octet.

5. Shapes
6. Polarity



Don’t forget the brackets for ions

Unsymmetrical Molecule
Therefore Dipolar

2 atoms, 2 lone pair
Bent – 109.5

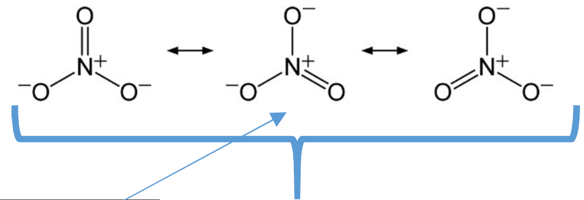
3 atoms, 0 lone pair
Trigonal Planar – 120

<u>Resonance Structures</u> occur when more than 1 correct Lewis Structure can be drawn for a molecule (having the same skeletal formula).

The molecule in nature is the average of the correct Lewis Structures.

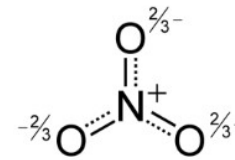
This is important because experimentally we observe the resonance structure, <u>not</u> the individual structures.

Resonance Structures (CHE 111 only)



The individual Lewis Structures for the NO_3^{-1} ion have 2 single bonds and 1 double bond. Theoretically we can measure the difference between the two.

However, experimentally, we see only 1 type of bond (represented by the hybrid structure).



<u>Formal Charges</u>

Dfn: A formal charge is the difference between the number of valence electrons an atom normally has and the number of electrons it has in a molecule.

Polyatomic ions result in atoms with Formal Charges

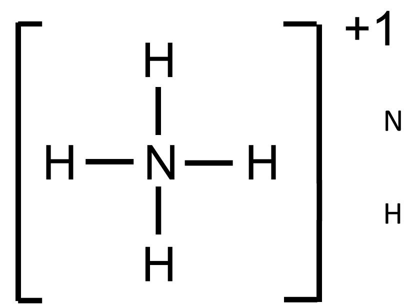
In cases where there is more than one correct Lewis Structure the one with the lowest FC is correct

Double Check: Sum FC = overall charge on ion

$$\textbf{Formal charge} = \begin{pmatrix}\text{number of valence}\\ \text{electrons in the}\\ \text{neutral atom}\end{pmatrix} - \underbrace{\begin{pmatrix}\text{number of valence}\\ \text{electrons around the}\\ \text{atom in the molecule}\end{pmatrix}}$$

$$\textbf{Formal charge} = \begin{pmatrix}\text{number of valence}\\ \text{electrons in the}\\ \text{neutral atom}\end{pmatrix} - \frac{1}{2}\begin{pmatrix}\text{number of electrons}\\ \text{in covalent bonds}\end{pmatrix} - \begin{pmatrix}\text{number of electrons}\\ \text{in lone pairs}\end{pmatrix}$$

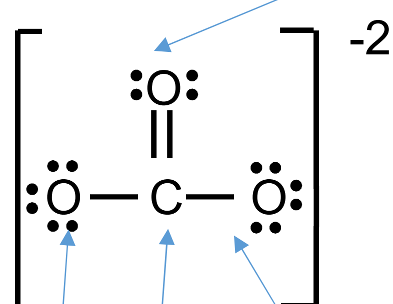
Formal Charges (CHE 111 only)



N: $5 - \frac{1}{2}(8) - 0 = +1$

H: $1 - \frac{1}{2}(2) - 0 = 0$

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



Double Check: The sum of the FC = -2 which is equal to the charge on the ion.

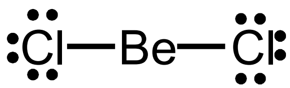
O: $6 - \frac{1}{2}(2) - 6 = -1$

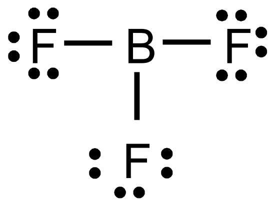
C: $4 - \frac{1}{2}(8) - 0 = 0$

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

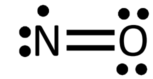
Violating the Octet Rule (CHE 111 only)

Incomplete Octets – molecules with fewer than 8 electrons can't complete octets but can still form molecules can form molecules. Generally occurs for Be and B.



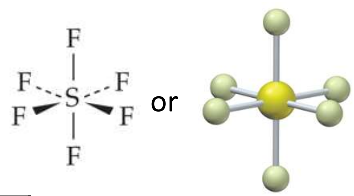


Odd Number of Electrons– molecules with an odd number of electrons are often called Free Radicals. They are very reactive and tend to be short lived.

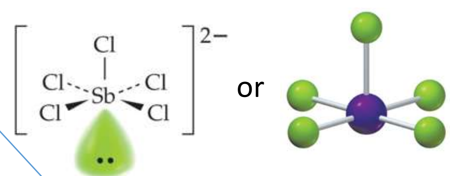


Expanded Octets: Elements in the 3rd row and below can access d-orbitals and have 12 (occasionally even 14) electrons. This generates 7 new shapes for molecules to have.

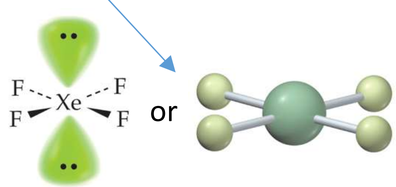
# atoms Bonded	# lone pairs	Shape	Bond Angle
6	0	Octahedral	90
5	1	Square Pyramidal	90
4	2	Square Planar	90



6 atoms, 0 lone pairs
Octahedral

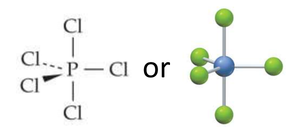


5 atoms, 1 lone pairs
Square Pyramidal

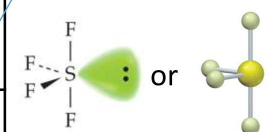


4 atoms, 2 lone pairs
Square Planar

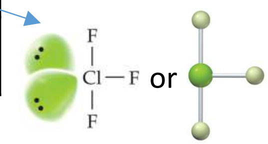
# atoms Bonded	# lone pairs	Shape	Bond Angle
5	0	Trigonal Bypyramidal	90 – Perp. 120 – In Plane
4	1	Seesaw	Complex
3	2	T-Shaped	90
2	0	Linear	180



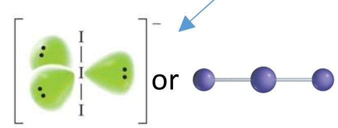
5 atoms, 0 lone pairs
Trigonal Pyramidal



4 atoms, 1 lone pairs
Seesaw



3 atoms, 2 lone pairs
T-Shape



2 atoms, 3 lone pairs
Linear