

Polarity, Formal Charge, and Resonance

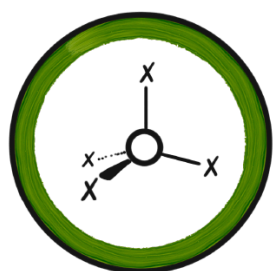
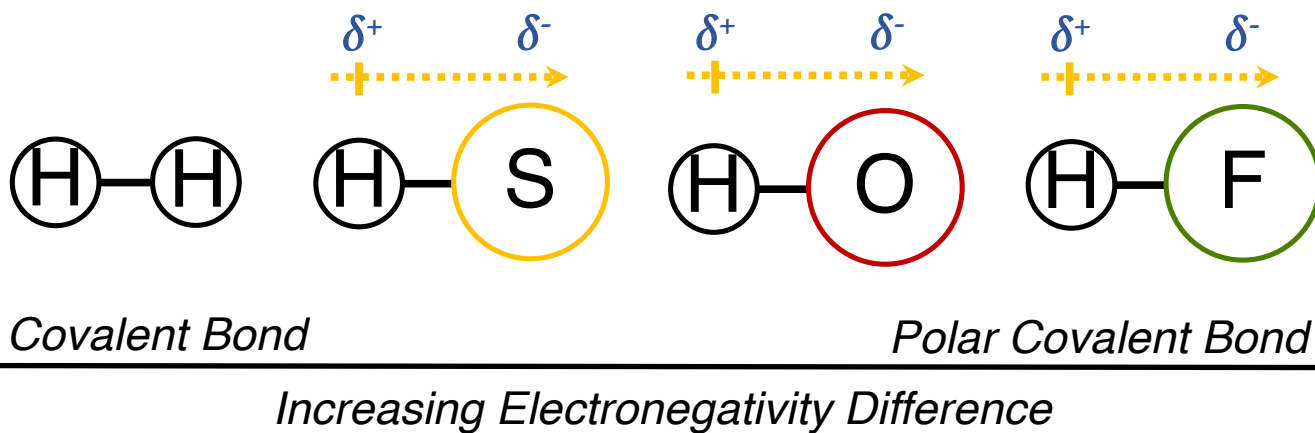
Flash Review

CHEM 371

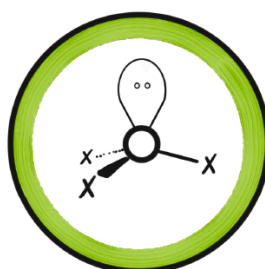
Dr. Christopher B. Durr



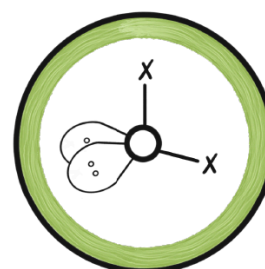
Polarity



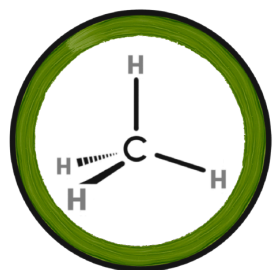
Tetrahedral



*Trigonal
Pyramid*

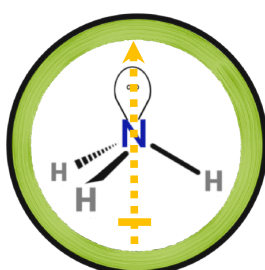


Bent



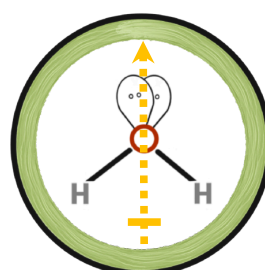
Methane

Non-Polar



Ammonia

Polar

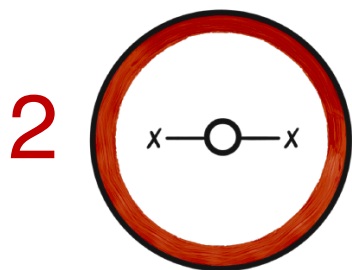


Water

Polar

Non-Polar

Bond dipoles are equivalent and cancel out

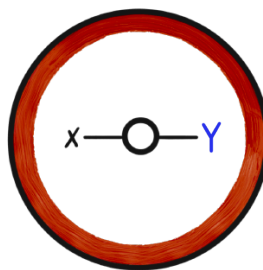


Linear

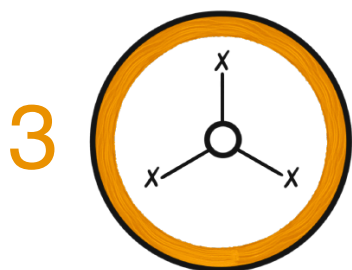


Polar

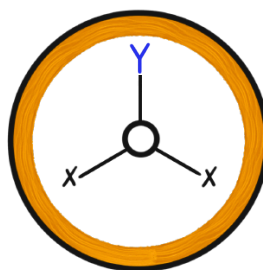
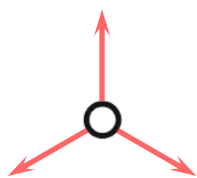
Bond dipoles are inequivalent and do not cancel out



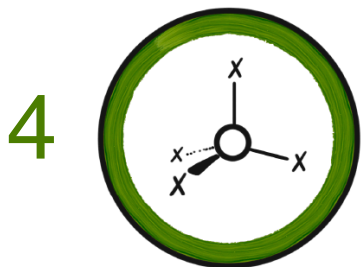
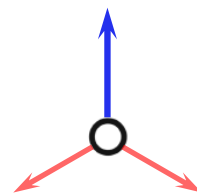
Linear



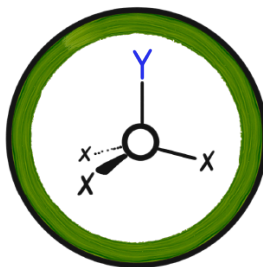
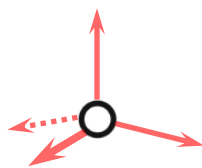
Trigonal Planar



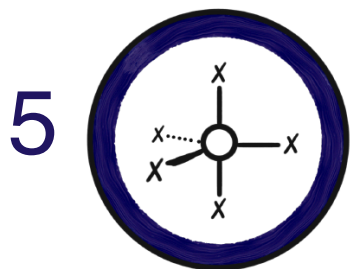
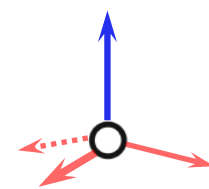
Trigonal Planar



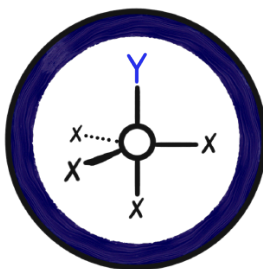
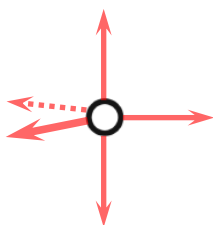
Tetrahedral



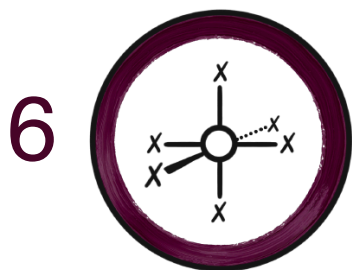
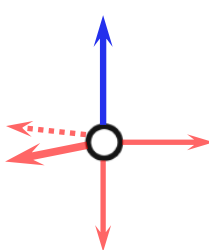
Tetrahedral



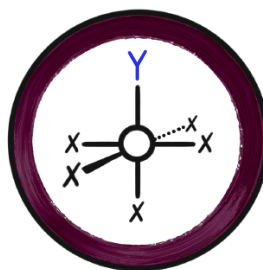
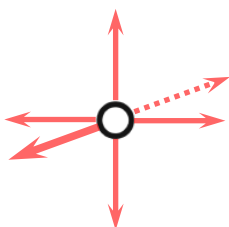
Trigonal Bipyramidal



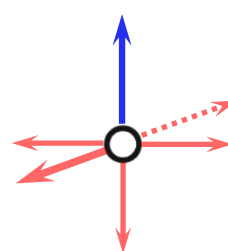
Trigonal Bipyramidal



Octahedral



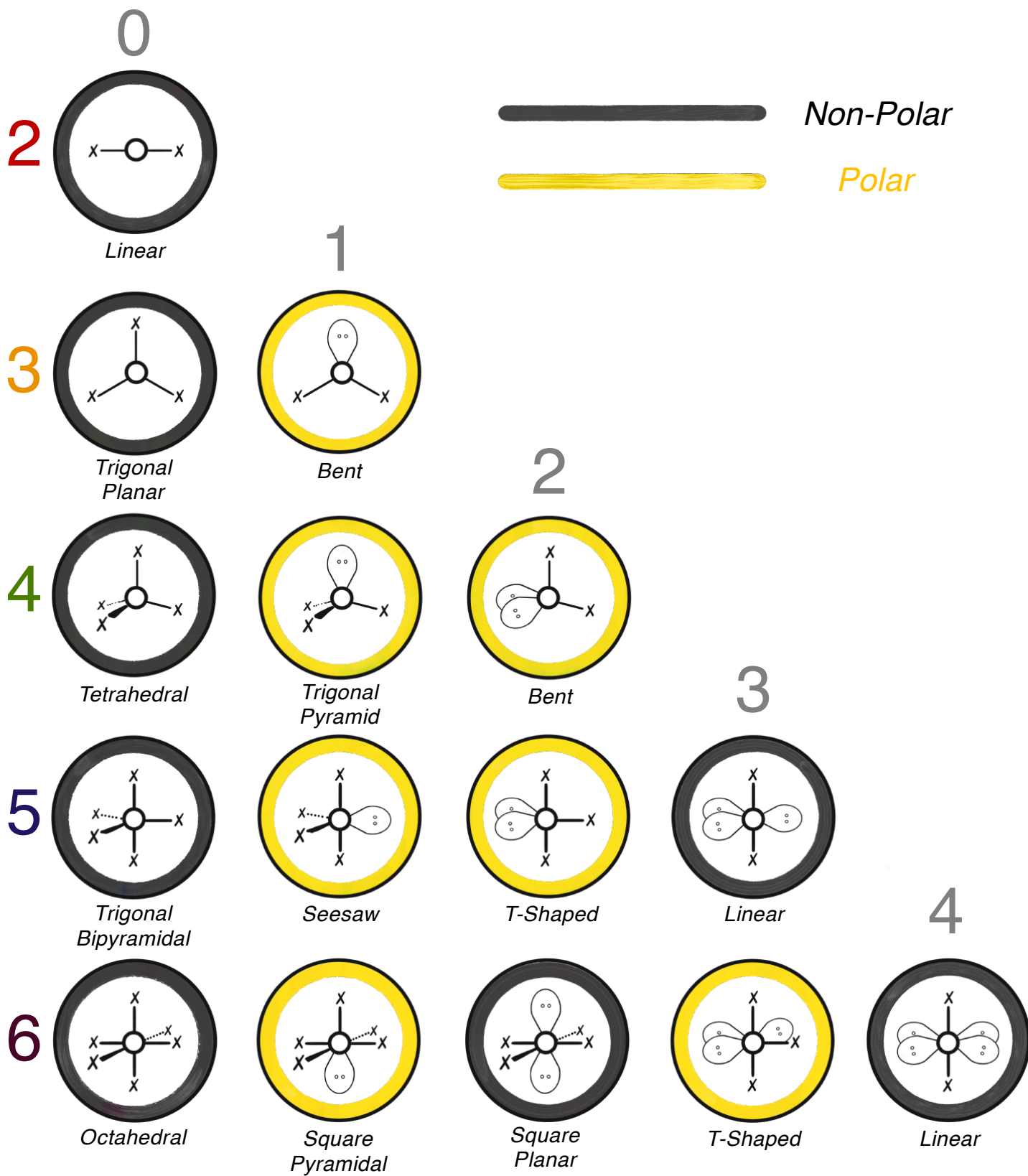
Octahedral



Polarity

Number of Lone Pairs

Steric Number



Non-Polar

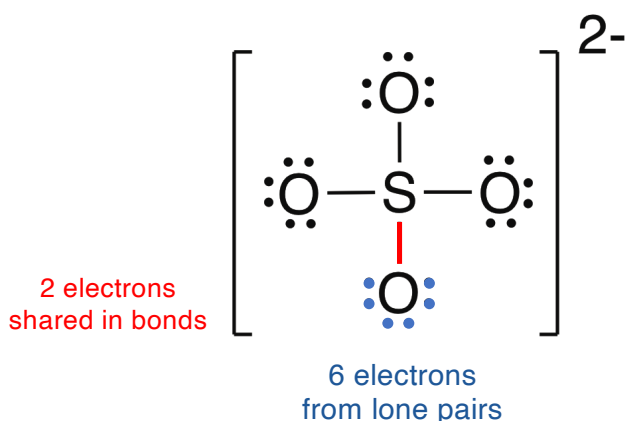


Polar

Calculating Formal Charge

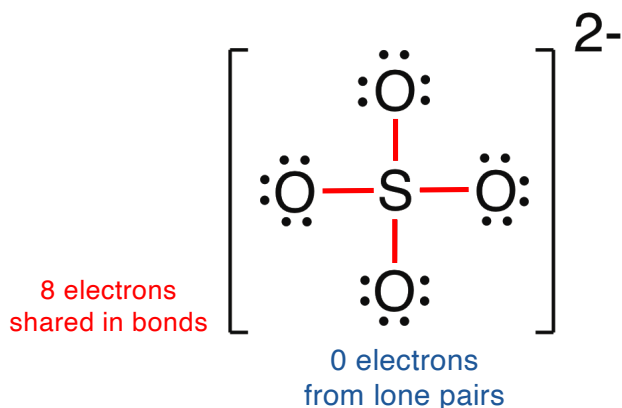
$$\text{Formal Charge} = \begin{array}{l} \# \text{ of electrons} \\ \text{in free atom} \end{array} - \begin{array}{l} \# \text{ of electrons} \\ \text{assigned in molecule} \end{array}$$

$$\begin{array}{l} \# \text{ of electrons} \\ \text{assigned in molecule} \end{array} = \begin{array}{l} \# \text{ of electrons} \\ \text{from lone pairs} \end{array} + \frac{1}{2} \begin{array}{l} \# \text{ of electrons} \\ \text{shared in bonds} \end{array}$$



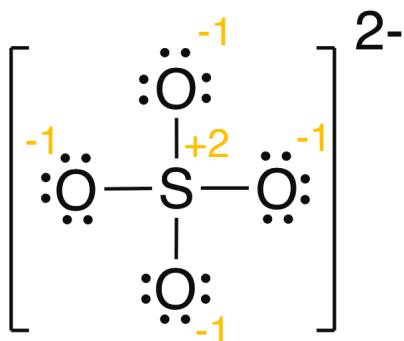
$$\text{F.C. (O)} = 6 - (6 + \frac{1}{2} (2))$$

$$\text{F.C. (O)} = -1$$



$$\text{F.C. (S)} = 6 - (0 + \frac{1}{2} (8))$$

$$\text{F.C. (S)} = +2$$



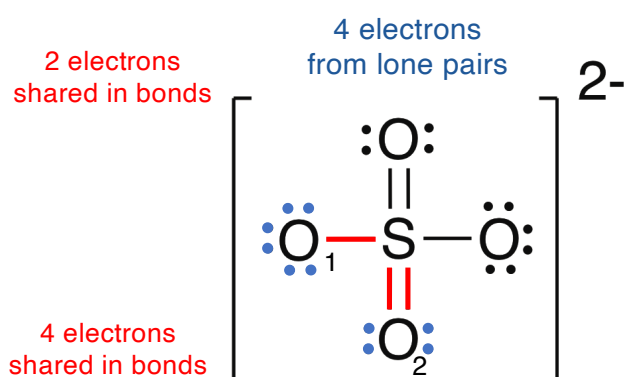
Sum of formal charges agrees with overall charge

Large Absolute Formal Charge

Calculating Formal Charge

$$\text{Formal Charge} = \begin{matrix} \text{\# of electrons} \\ \text{in free atom} \end{matrix} - \begin{matrix} \text{\# of electrons} \\ \text{assigned in molecule} \end{matrix}$$

$$\begin{matrix} \text{\# of electrons} \\ \text{assigned in molecule} \end{matrix} = \begin{matrix} \text{\# of electrons} \\ \text{from lone pairs} \end{matrix} + \frac{1}{2} \begin{matrix} \text{\# of electrons} \\ \text{shared in bonds} \end{matrix}$$

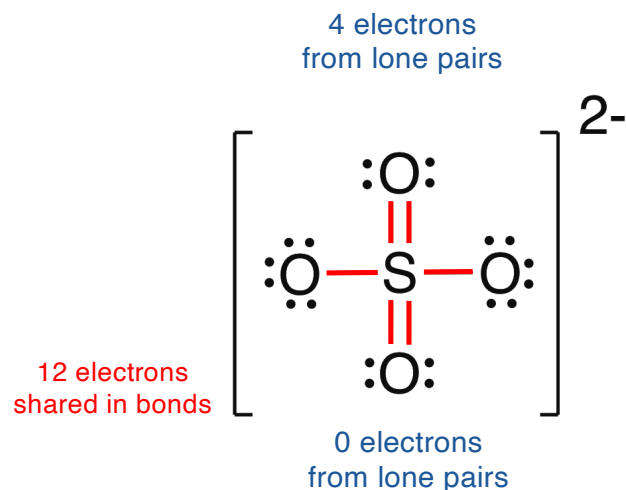


$$\text{F.C. (O}_1) = 6 - (6 + \frac{1}{2} (2))$$

$$\text{F.C. (O}_1) = -1$$

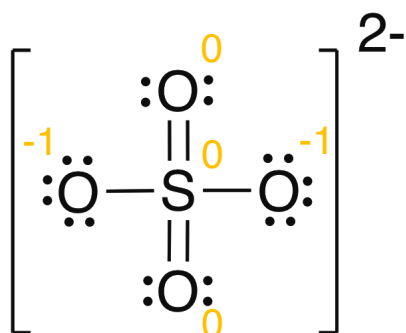
$$\text{F.C. (O}_2) = 6 - (4 + \frac{1}{2} (4))$$

$$\text{F.C. (O}_2) = 0$$



$$\text{F.C. (S)} = 6 - (0 + \frac{1}{2} (12))$$

$$\text{F.C. (S)} = 0$$

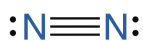
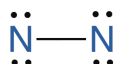


Sum of formal charges agrees with overall charge

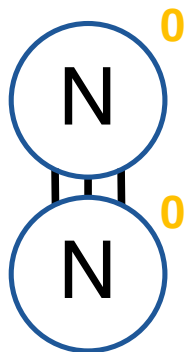
Reduced Formal Charge

Examples of Formal Charge

N_2

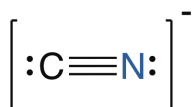
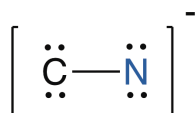


$$N = 5 - (2 + \frac{1}{2}(6)) = 0$$



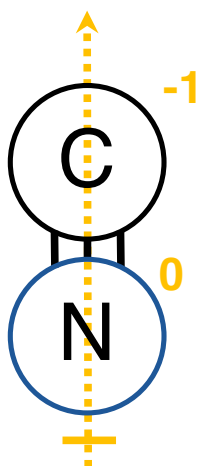
No Net Dipole

CN^-



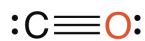
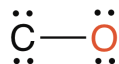
$$N = 5 - (2 + \frac{1}{2}(6)) = 0$$

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



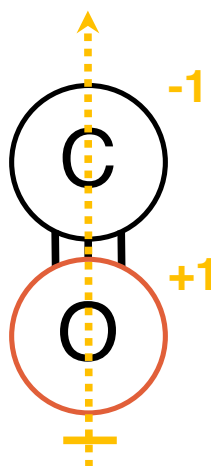
Dipole Towards C

CO



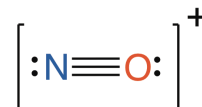
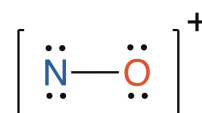
$$C = 4 - (2 + \frac{1}{2}(6)) = -1$$

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



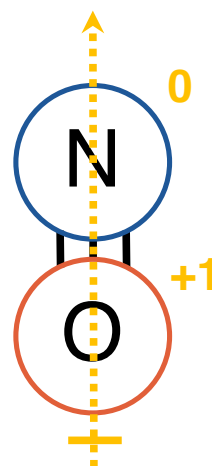
Dipole Towards C

NO^+



$$N = 5 - (2 + \frac{1}{2}(6)) = 0$$

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



Dipole Towards N

Resonance

Resonance Hybrids result from two or more **Resonance Contributors**.

Please note, electrons are *not* shifting back and forth, this is importantly *not* an interconverting equilibrium.

