

FORMAL CHARGE

- You can often draw more than one structure for a molecule that appears correct. How can you determine which one is more likely?

- USE FORMAL CHARGE!

- Formal charge is a hypothetical charge on each atom in a structure. It assumes:

- ① All bonding electrons are shared EQUALLY between atoms
- ② Lone pairs are NOT shared.

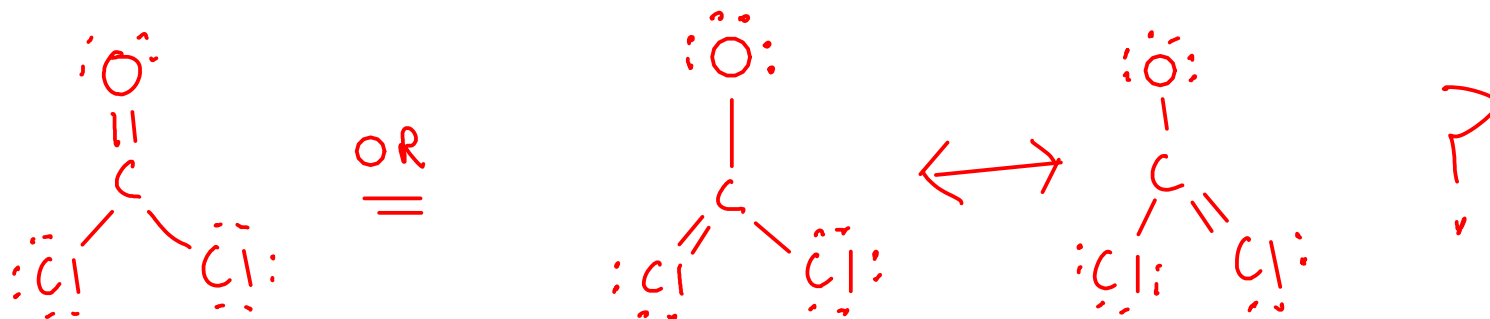
$$\text{FORMAL CHARGE} = \text{ORIGINAL \# OF VALENCE ELECTRONS} - \text{NUMBER OF BONDS} - \text{NUMBER OF UNSHARED ELECTRONS}$$

* The sum of the formal charges of all atoms in a structure should equal to the charge of the molecule (0 for neutral molecules)

The "better" Lewis structure will have:

- Lower magnitudes of formal charge (0 is better than +2 -2)
- Negative formal charges on ELECTRONEGATIVE atoms, or positive formal charges on atoms that are less electronegative.

EXAMPLE: COCl_2



... calculate formal charges to tell which structure is more likely!

$$\text{O}: 6 - 2 - 4 = 0$$

$$\text{C}: 4 - 4 - 0 = 0$$

$$\text{Cl}: 7 - 1 - 6 = 0$$

$$\text{Cl}: 7 - 1 - 6 = 0$$

$$\text{O}: 6 - 1 - 6 = -1$$

$$\text{C}: 4 - 4 - 0 = 0$$

$$=\text{Cl}: 7 - 2 - 4 = +1$$

$$-\text{Cl}: 7 - 1 - 6 = 0$$

* Based on FORMAL CHARGE, we would pick the structure on the left as the actual structure of the molecule - lower formal charges (all 0) than the structure on the right.



... we can determine which of these structures is more likely by calculating formal charges!

$$\text{H}: 1 - 1 - 0 = 0$$

$$\text{C}: 4 - 3 - 2 = -1$$

$$\text{N}: 5 - 4 - 0 = +1$$

$$\text{H}: 1 - 1 - 0 = 0$$

$$\text{C}: 4 - 4 - 0 = 0$$

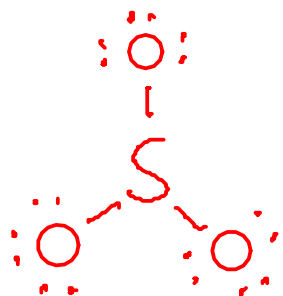
$$\text{N}: 5 - 3 - 2 = 0$$

Which structure is more likely?

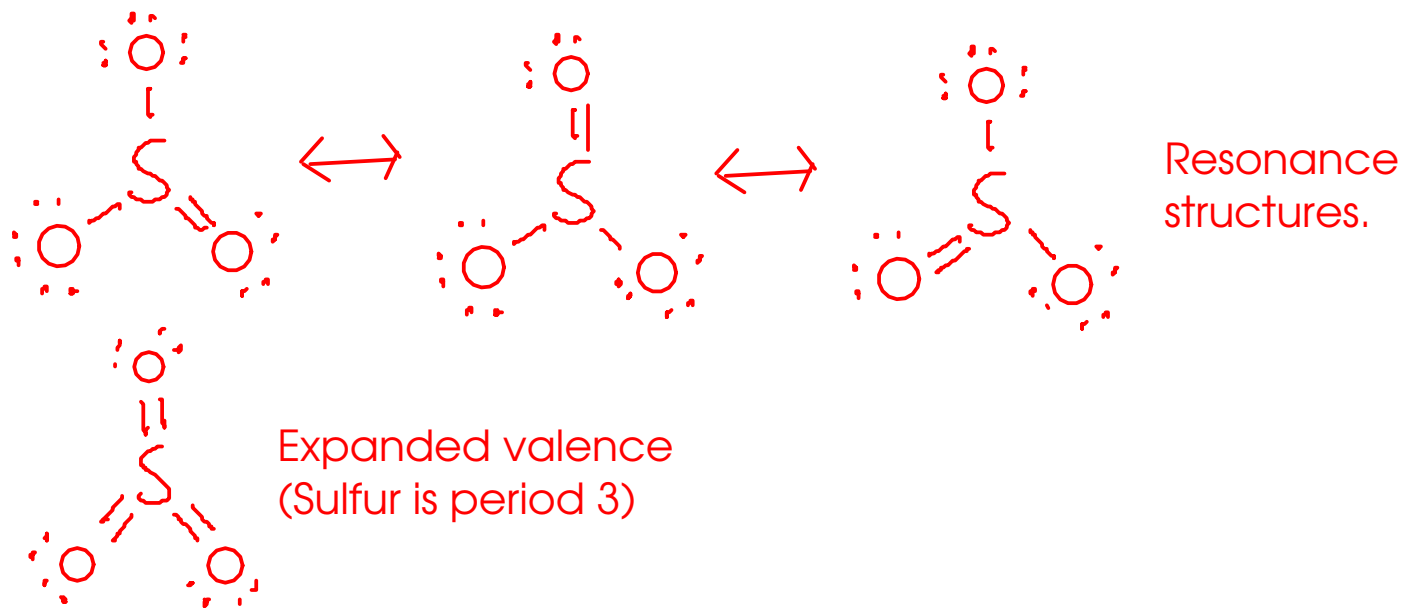
- * Based on FORMAL CHARGE, the HCN structure is more likely. It has lower formal charges than the HNC structure.
- * The HNC structure places a positive formal charge on electronegative N, while at the same time it gives carbon a negative formal charge.

Let's look at sulfur trioxide. SO_3

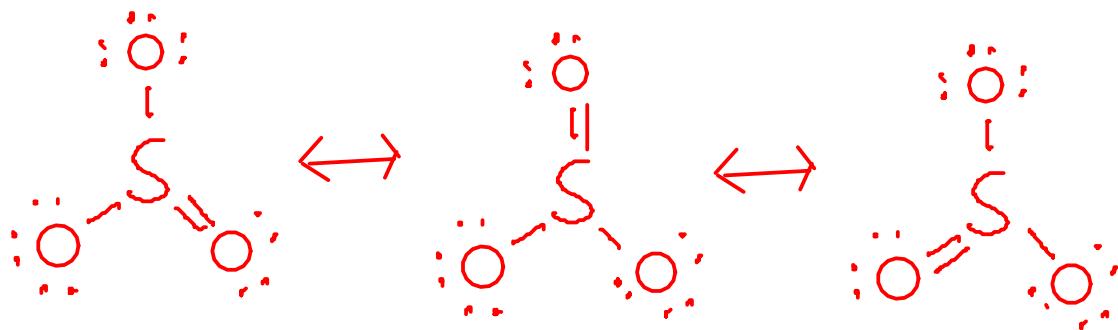
Skeletal structure:



$$\begin{array}{r} \text{S: } 6 \\ \text{O: } 6 \times 3 = 18 \\ \hline 24 e^- \end{array}$$

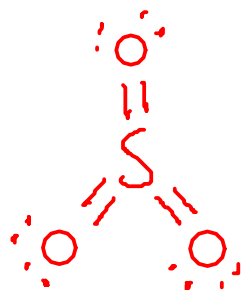


To decide which structure is preferred, let's look at formal charges.



Resonance structures.

$$\begin{aligned} \text{S: } & 6 - 4 - 0 = +2 \\ \text{O-: } & 6 - 1 - 6 = -1 \\ \text{O-: } & 6 - 1 - 6 = -1 \\ \text{O=: } & 6 - 2 - 4 = 0 \end{aligned}$$



Expanded valence
(Sulfur is period 3)

$$\begin{aligned} \text{S: } & 6 - 6 - 0 = 0 \\ \text{O=: } & 6 - 2 - 4 = 0 \\ \text{O=: } & 6 - 2 - 4 = 0 \\ \text{O=: } & 6 - 2 - 4 = 0 \end{aligned}$$

BASED ON FORMAL CHARGE, the expanded valence structure of sulfur trioxide is the most likely one.

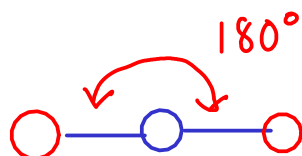
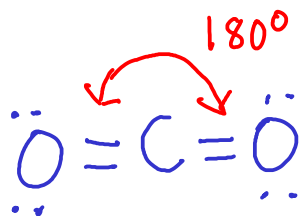
The correct (as in, agrees with experiment) structure is TYPICALLY the one with minimized formal charge - EVEN IF the structure violates the octet rule.

Remember, though, that Period 2 atoms like carbon NEVER end up with more than eight valence electrons!

The shape of simple molecules (and parts of larger molecules) can be easily predicted using the VSEPR model

VSEPR = Valence Shell Electron Pair Repulsion Model

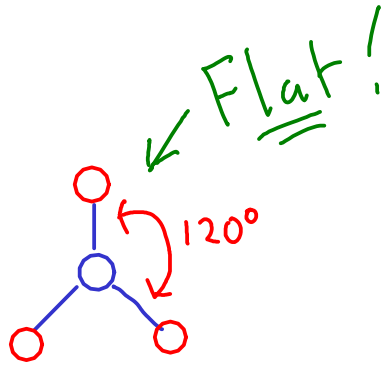
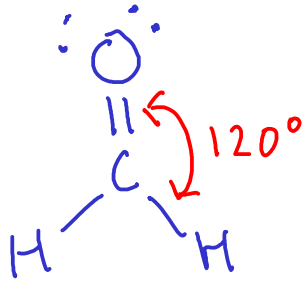
- Each BOND or LONE PAIR OF ELECTRONS around an atom will try to move itself as far away from other bonds or lone pairs as possible!



For the two red circles to be farthest apart, they must be 180 degrees apart

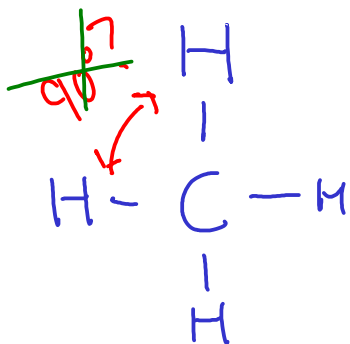
LINEAR
MOLECULES

ANY diatomic (two-atom) molecule is linear, but only some three-atom molecules are!



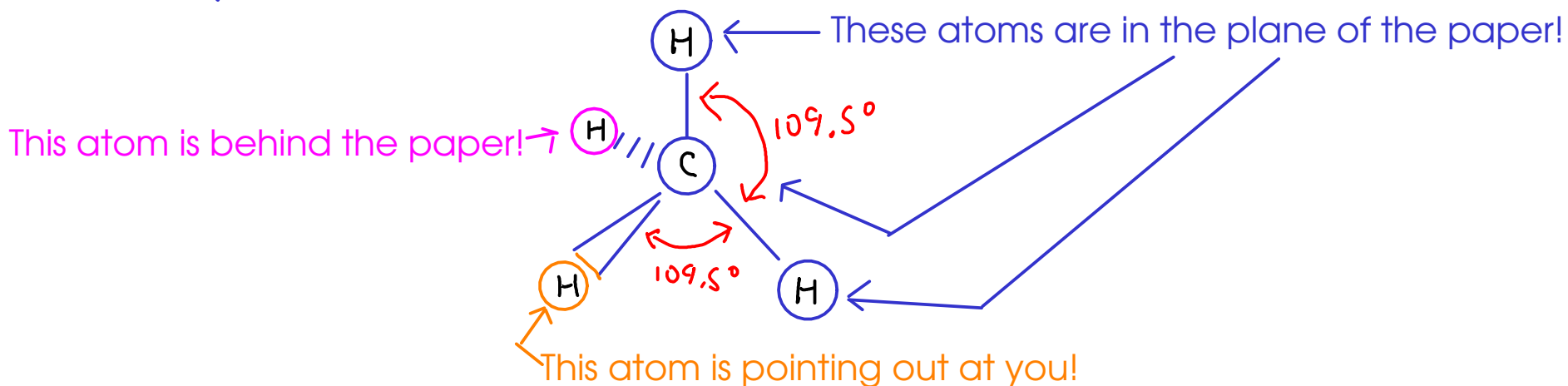
For the three red circles to be farthest apart, they spread out so that each is 120 degrees from the others!

TRIGONAL
PLANAR
MOLECULES



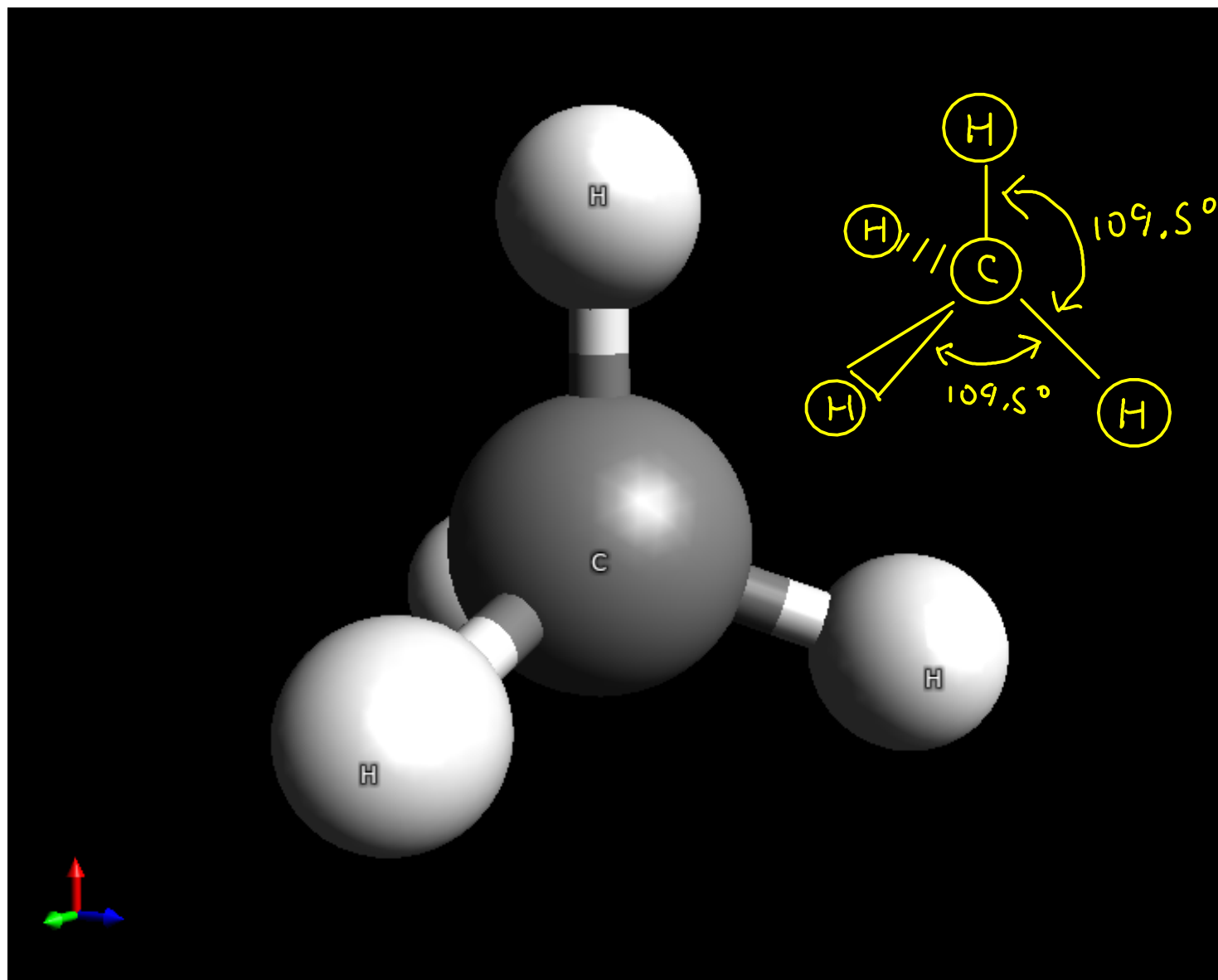
These hydrogen atoms might appear at first glance to be 90 degrees apart, but remember that molecules exist in THREE DIMENSIONS, not two!

Each hydrogen atom is actually 109.5 degrees apart, forming a TETRAHEDRON.



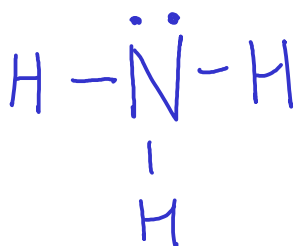
To see the tetrahedron in three dimensions WITHOUT buying a molecular model kit, just take four balloons, blow them up, and then tie them together. The knot will be the central atom, and the balloons will line themselves up to be 109.5 degrees apart.

Here's a computer ball-and-stick rendering of the methane molecule.



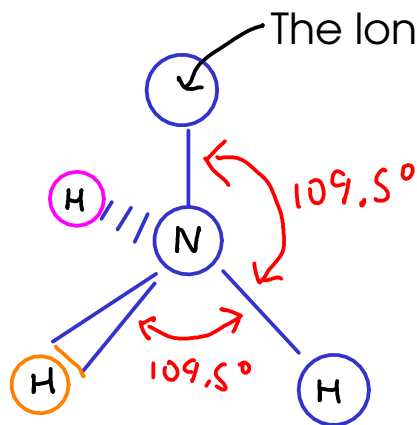
DERIVATIVES OF THE TETRAHEDRON

- What if there are lone pairs? The way the shape of a molecule is described depends on the ATOMS in the molecule, even though lone pairs play a role in the positions of the atoms.

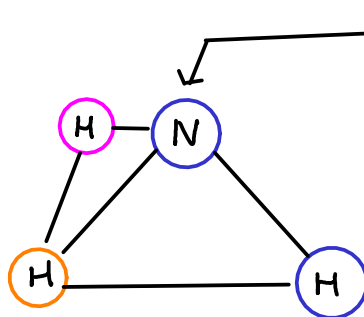


Since there are four "things" around the nitrogen atom, we would expect them to be approximately 109.5 degrees apart (in other words, TETRAHEDRAL). BUT ... only three of these things are atoms.

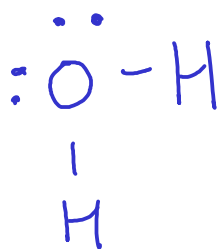
The atoms are arranged in a PYRAMID shape, so we call this molecule PYRAMIDAL!



The lone pair takes one position in the tetrahedron



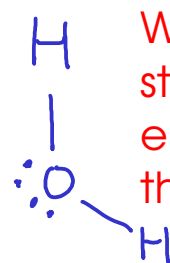
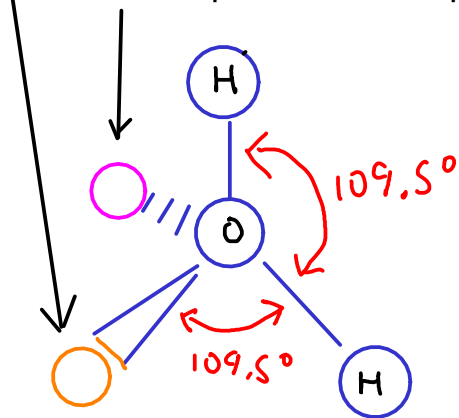
By just looking at the atoms, you can see the pyramid - with the central nitrogen atom as the top and the hydrogen atoms forming the base of the pyramid.



Since there are four "things" around the oxygen atom, we would expect them to be approximately 109.5 degrees apart (in other words, TETRAHEDRAL). BUT... only two of these things are atoms.

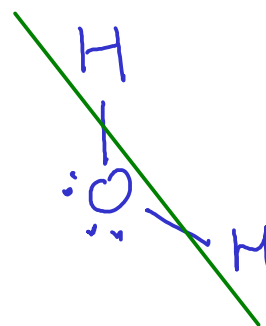
The atoms are all in a single plane, but they are not lined up in a straight line. We call this shape "BENT".

Lone pairs take up two positions in the tetrahedron



We sometimes draw the Lewis structure of water this way to emphasize the "bent" nature of the molecule!

Notice that this molecule has two "sides", one with the oxygen atom and one with hydrogen atoms.



* These atoms are in the same plane, like carbon dioxide. But they are not arranged linearly!