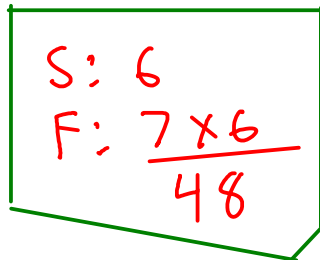
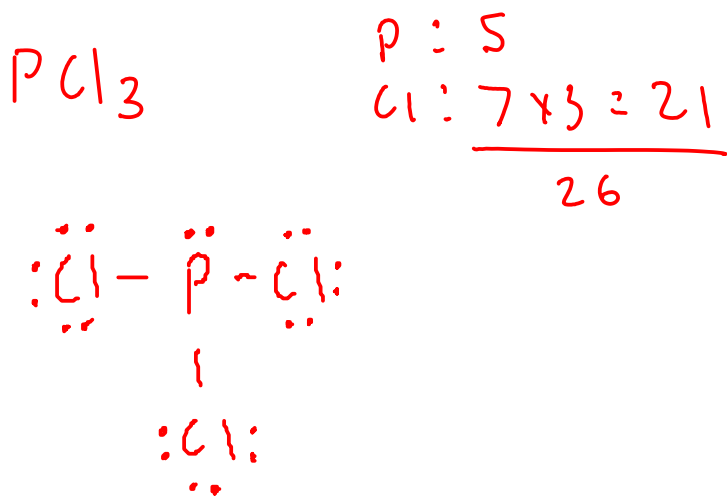


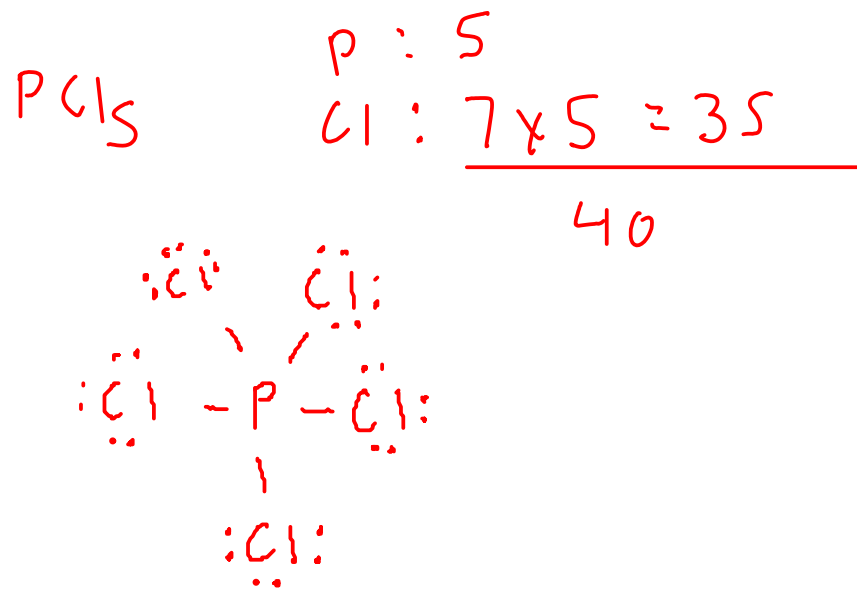
EXAMPLES:



- The central SULFUR atom has a share in TWELVE total electrons, not eight!
- The SHAPE of the sulfur hexafluoride molecule in three dimensions agrees with the picture of six fluorine atoms each sharing a pair of electrons with a sulfur center.

PCl₃ vs PCl₅

This structure obeys the octet rule.



This molecule does NOT obey the octet rule. Phosphorus ends up with ten electrons instead of eight.

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.

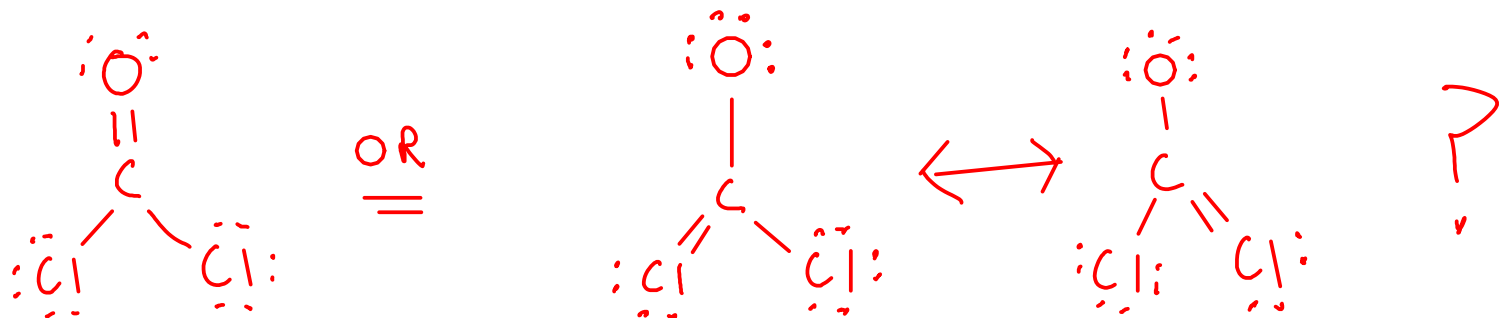
$$\text{FORMAL CHARGE} = \text{ORIGINAL \# OF VALENCE ELECTRONS} - \text{NUMBER OF BONDS} - \text{NUMBER OF UNSHARED ELECTRONS}$$

* 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 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!

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

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

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

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

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

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

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

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

* The sum of all formal charges on BOTH the proposed structures equals zero, so they have been drawn correctly. This is a neutral molecule.

* Based on formal charges, the structure on the left is preferred, since it has LOWER formal charges (all 0) than the structure on the right (+1/-1/0)



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

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

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

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

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

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

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

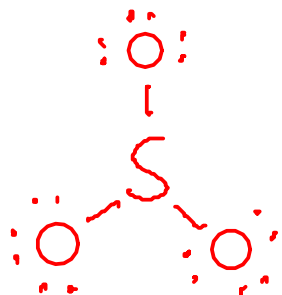
Which structure is more likely?

* Based on formal charges, the HCN structure (on the right) is more likely. It has lower formal charges than the HNC structure on left does.

(Also, the HNC structure places a positive formal charge on NITROGEN, while CARBON gets a negative formal charge)

Let's look at sulfur trioxide. SO_3

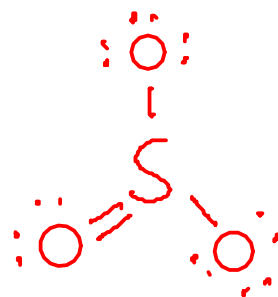
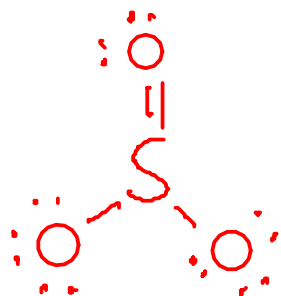
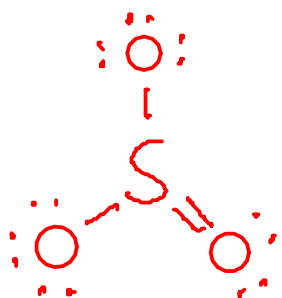
Skeletal structure:



$$\text{S} : 6$$

$$\text{O} : 6 \times 3 = 18$$

$$24 e^-$$

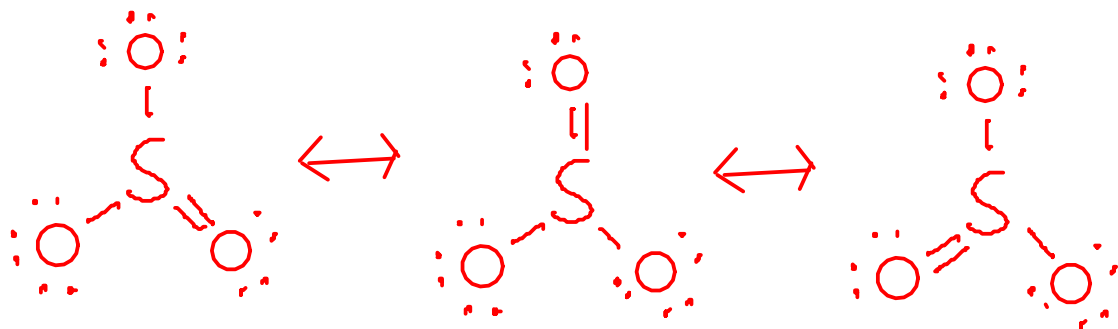


Resonance structures.



Expanded valence
(Sulfur is period 3)

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



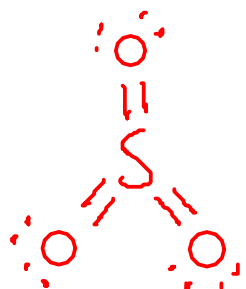
Resonance structures.

$$S: 6 - 4 - 0 = +2$$

$$O-: 6 - 1 - 6 = -1$$

$$O-: 6 - 1 - 6 = -1$$

$$O=: 6 - 2 - 4 = 0$$



Expanded valence
(Sulfur is period 3)

$$S: 6 - 6 - 0 = 0$$

$$O=: 6 - 2 - 4 = 0$$

$$O=: 6 - 2 - 4 = 0$$

$$O=: 6 - 2 - 4 = 0$$

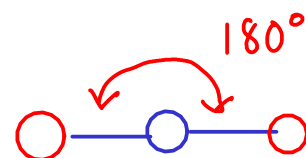
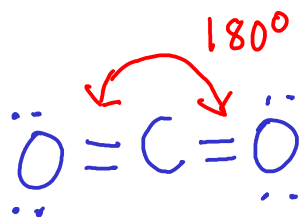
BASED ON FORMAL CHARGES, we prefer the expanded valence structures to the resonance structures.

(The correct structure is usually the one with lower formal charges EVEN IF that structure violates the octet rule. Just remember that period 2 atoms never end up with more than eight outer-shell 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

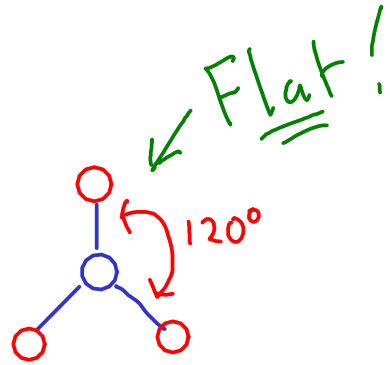
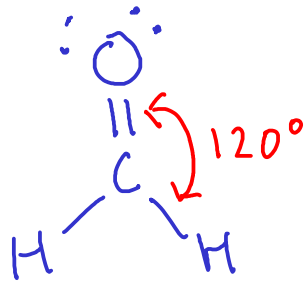
- Each BOND or LONE PAIR OF ELECTRONS around an atom will try to move itself as far away from other bonds or lone pairs as possible!



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

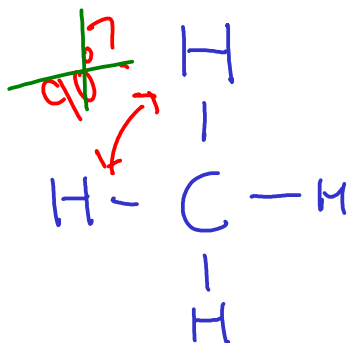
LINEAR
MOLECULES

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



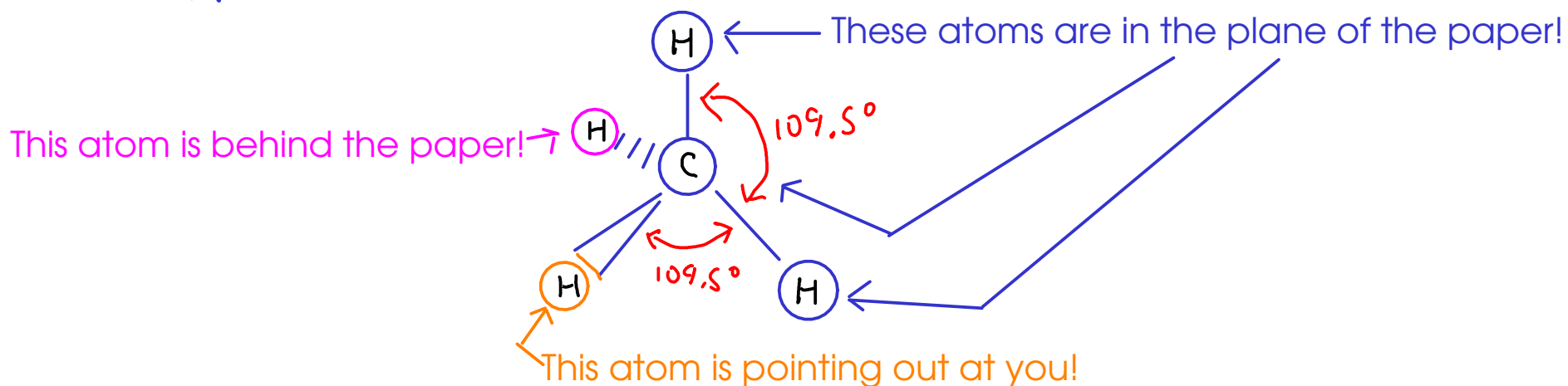
For the three red circles to be farthest apart, they spread out so that each is 120 degrees from the others!

TRIGONAL
PLANAR
MOLECULES



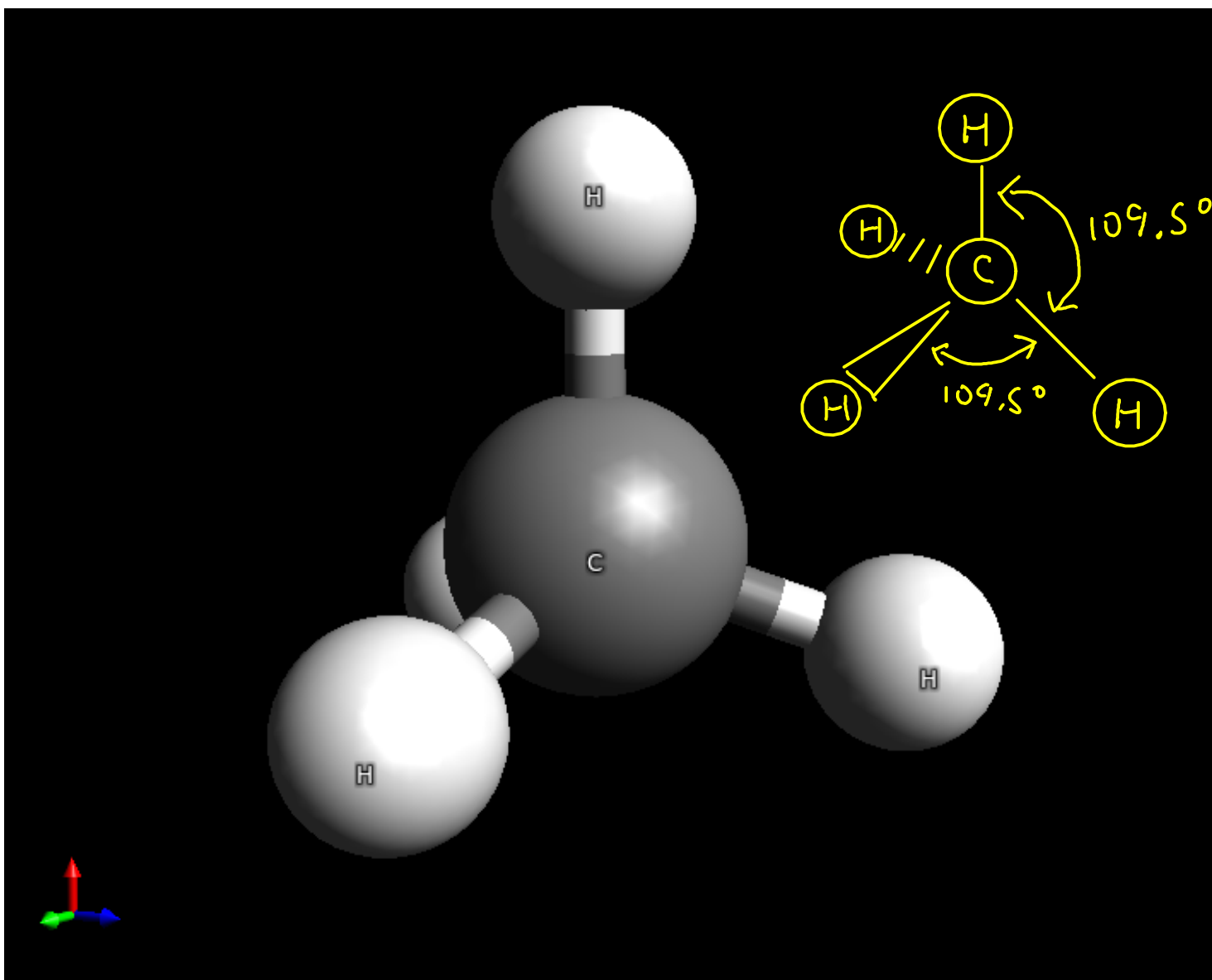
These hydrogen atoms might appear at first glance to be 90 degrees apart, but remember that molecules exist in THREE DIMENSIONS, not two!

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



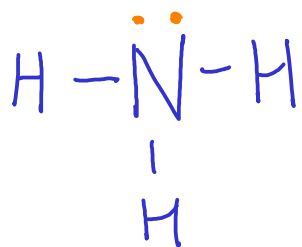
To see the tetrahedron in three dimensions WITHOUT buying a molecular model kit, just take four balloons, blow them up, and then tie them together. The knot will be the central atom, and the balloons will line themselves up to be 109.5 degrees apart.

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



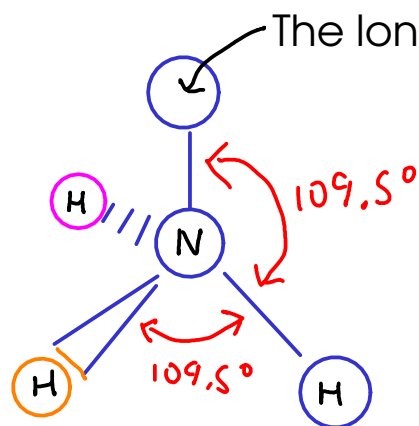
DERIVATIVES OF THE TETRAHEDRON

- 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.

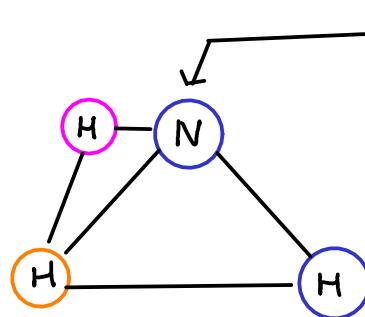


Since there are four "things" around the nitrogen atom, we would expect them to be approximately 109.5 degrees apart (in other words, TETRAHEDRAL). BUT ... only three of these things are atoms.

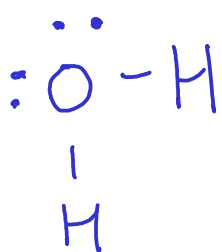
The atoms are arranged in a PYRAMID shape, so we call this molecule PYRAMIDAL!



The lone pair takes one position in the tetrahedron



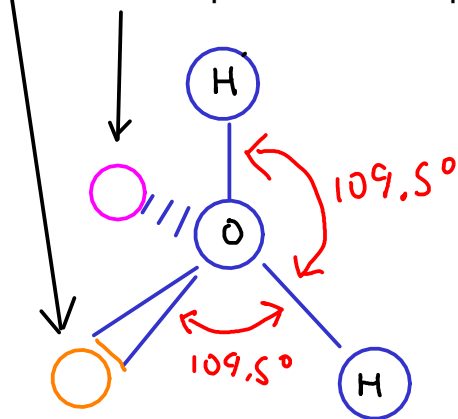
By just looking at the atoms, you can see the pyramid - with the central nitrogen atom as the top and the hydrogen atoms forming the base of the pyramid.



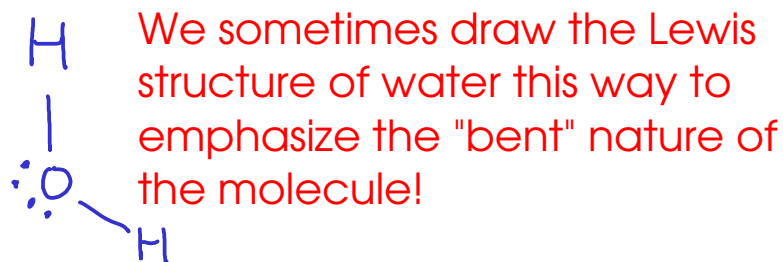
Since there are four "things" around the oxygen atom, we would expect them to be approximately 109.5 degrees apart (in other words, TETRAHEDRAL). BUT... only two of these things are atoms.

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

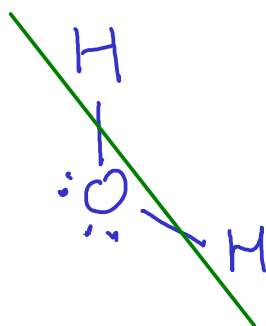


* These atoms are in the same plane, like carbon dioxide. But they are not arranged linearly!

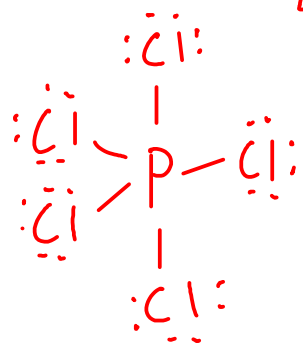
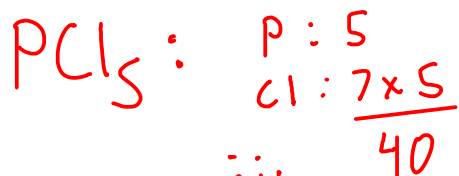


We sometimes draw the Lewis structure of water this way to emphasize the "bent" nature of the molecule!

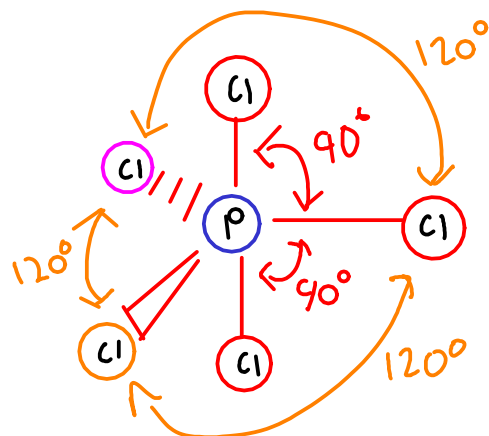
Notice that this molecule has two "sides", one with the oxygen atom and one with hydrogen atoms.



SHAPES OF EXPANDED VALENCE MOLECULES

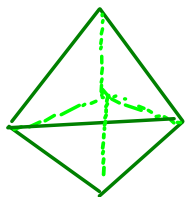


There are five atoms bonded to the central phosphorus atom, and they will attempt to get as far apart as possible from one another!



The top and bottom atoms are 90 degrees apart from the atoms around the center.

The atoms around the center are 120 degrees apart from each other.

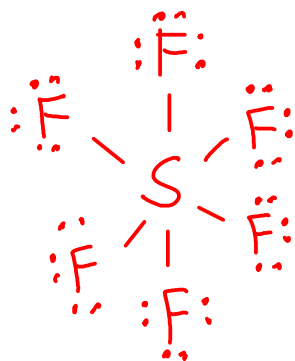


There are actually two DIFFERENT bond angles in this structure. It's called TRIGONAL BIPYRAMIDAL.

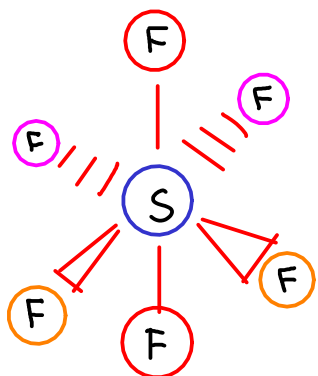
There are several derivatives of the trigonal bipyramidal shape (like the tetrahedral shape) - depending on how many things around the central atom are atoms!



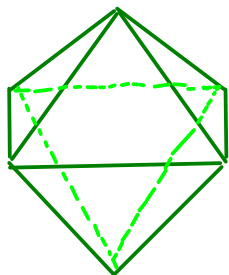
$$\begin{array}{l} S: 6 \\ F: 7 \times 6 \\ \hline 48 \end{array}$$



There are six atoms bonded to the central sulfur atom, and they will attempt to get as far apart as possible from one another!



All bond angles in this arrangement are 90 degrees!



This shape is called OCTAHEDRAL, since it has eight sides.

Like the tetrahedral and trigonal bipyramidal arrangements, there are several derivatives of the octahedron - depending on how many of the six things around the center are atoms!

Here's a ball-and-stick rendering of the sulfur hexafluoride molecule:

