

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.

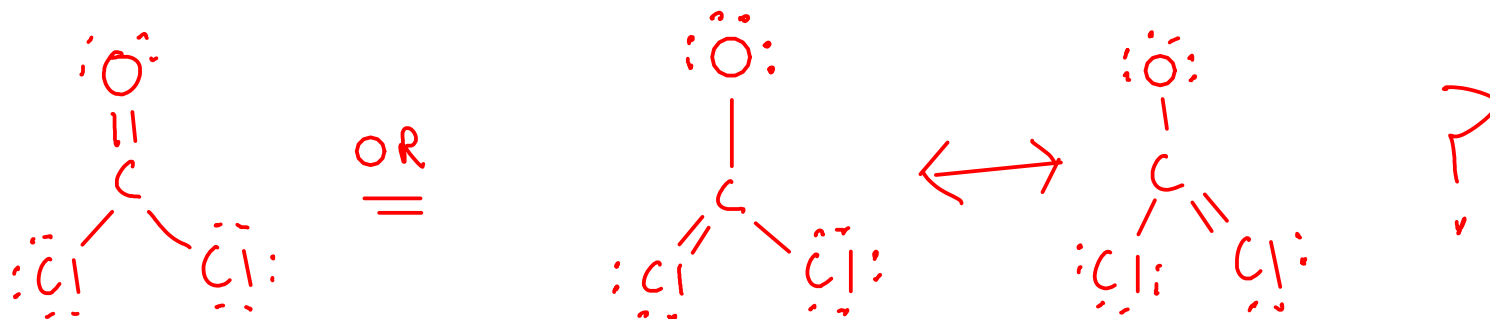
$$\text{FORMAL CHARGE} = \text{ORIGINAL \# OF VALENCE ELECTRONS} - \text{NUMBER OF BONDS} - \text{NUMBER OF UNSHARED ELECTRONS}$$

* 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!

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

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

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

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

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

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

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

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

The structure on the LEFT is preferred. It has lower formal charges than the structure on the right.



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

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

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

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

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

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

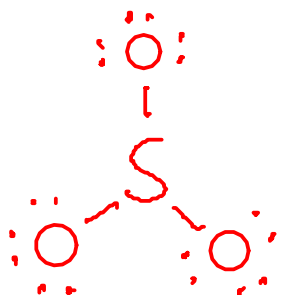
$$\text{N}: 5 - 3 - 2 = 0$$

Which structure is more likely?

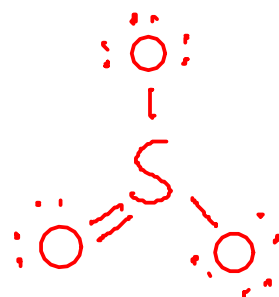
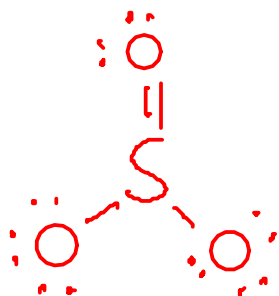
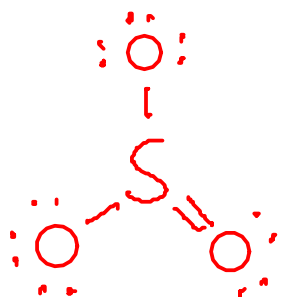
- * The HCN structure is more likely. It has lower formal charges than the HNC structure does.
- * the HNC structure has another problem. It puts a positive formal charge on the nitrogen atom, while putting a negative formal charge on the much less electronegative carbon atom.

Let's look at sulfur trioxide. SO_3

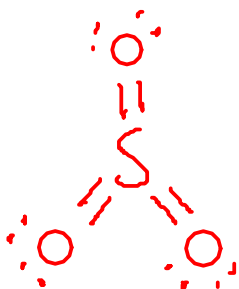
Skeletal structure:



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

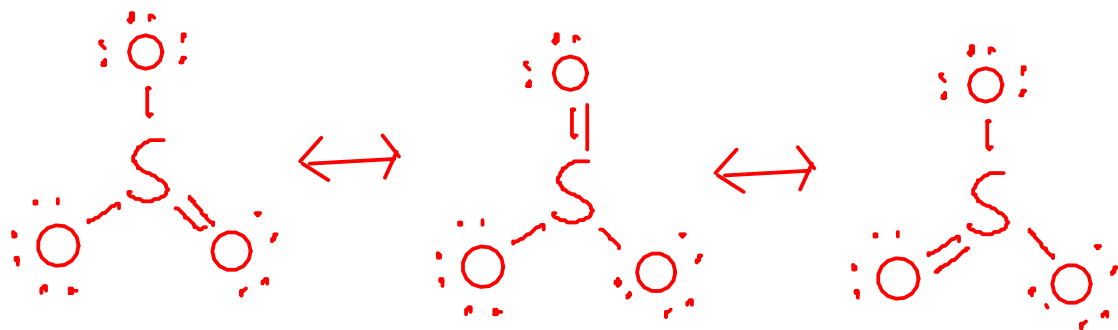


Resonance structures.



Expanded valence
(Sulfur is period 3)

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



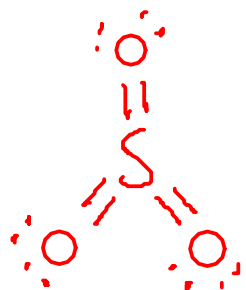
Resonance structures.

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

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

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

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



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, the expanded valence structure is the more likely one.

The correct (as in - agrees with experimental information about the compound) structure is USUALLY the one preferred by formal charge, even if the structure violates the octet rule. (Remember, though, that period 2 can't have more than eight electrons!)

Experimental evidence for sulfur trioxide suggests that the bond lengths are closest to double bond length.