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.

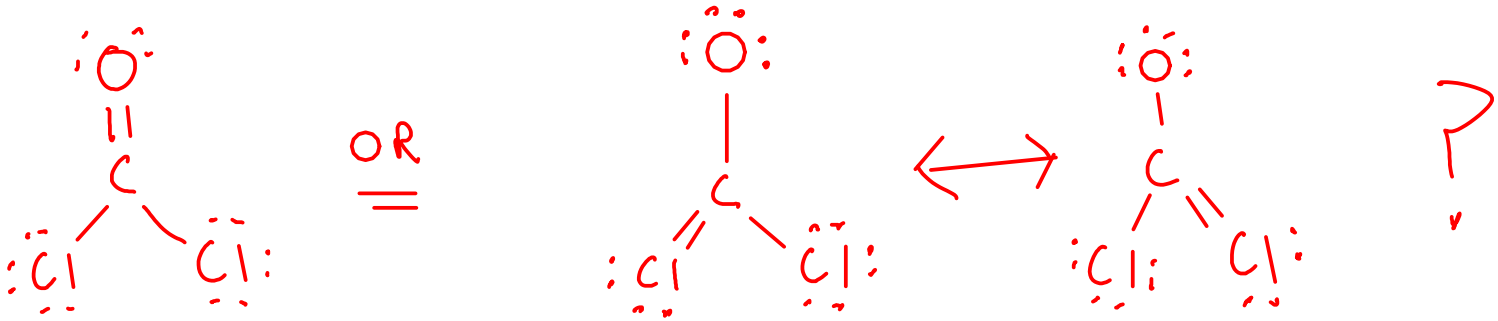
FORMAL CHARGE = ORIGINAL # OF VALENCE ELECTRONS − NUMBER OF BONDS − NUMBER OF UNSHARED ELECTRONS

* 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!

O: 6 − 2 − 4 = 0

C: 4 − 4 − 0 = 0

Cl: 7 − 1 − 6 = 0

Cl: 7 − 1 − 6 = 0

O: 6 − 1 − 6 = −1

C: 4 − 4 − 0 = 0

= Cl: 7 − 2 − 4 = +1

− Cl: 7 − 1 − 6 = 0

Based on formal charges, the structure on the LEFT is preferred,. since 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!

H: 1 – 1 – 0 = 0

C: 4 – 3 – 2 = –1

N: 5 – 4 – 0 = +1

H: 1 – 1 – 0 = 0

C: 4 – 4 – 0 = 0

N: 5 – 3 – 2 = 0

Which structure is more likely?

* The HCN structure is more likely. It has lower formal charges than the HNC strcuture.

* The HNC structure has another problem. It puts a positive formal charge on NITROGEN, while the carbon connected to it has a NEGATIVE formal charge - implying that the carbon is pulling electrons away from nitrogen. Since nitrogen is the more electronegative of the two, this is unlikely.

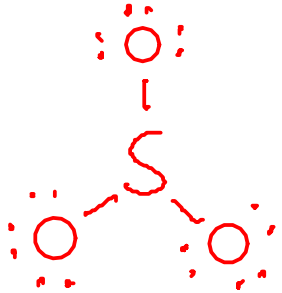
Let's look at sulfur trioxide. SO_3

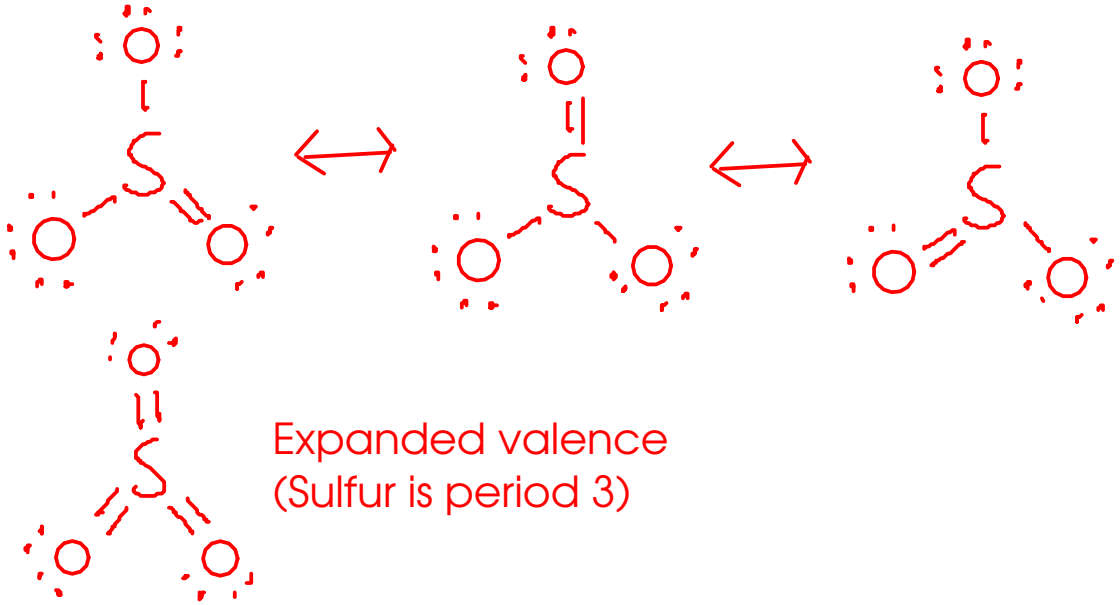
S: 6

O: 6 x 3 = 18

24 e⁻

Skeletal structure:

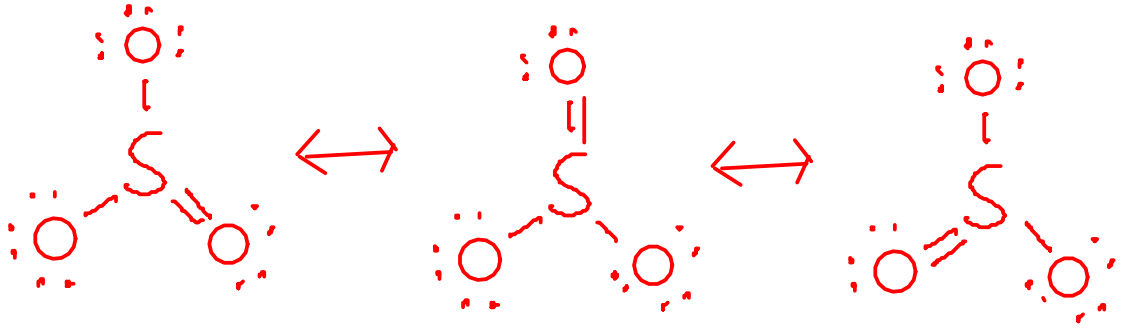




Resonance structures.

Expanded valence
(Sulfur is period 3)

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



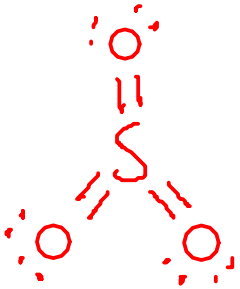
Resonance structures.

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 for sulfur trioxide is most likely.

The correct structure is usually the one with lowest formal charge, even if that structure violates the octet rule. (Remember, though, that certain atoms can't end up with more than eight electrons - the members of Period 2!)