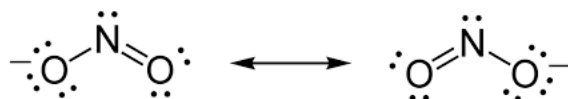


Resonance and Formal Charges

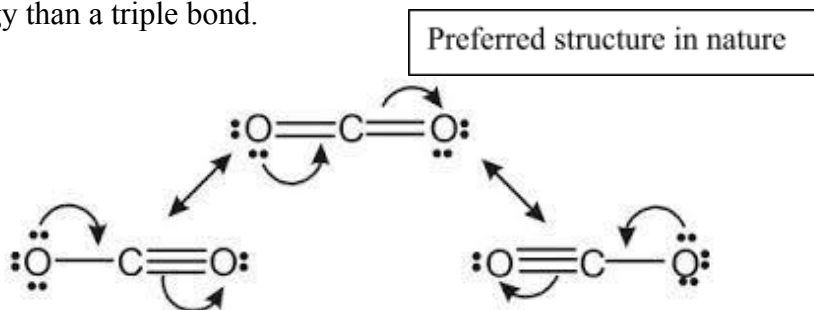
Resonance occurs when two or more structures can be drawn for a molecule with their atoms in the same attachments. It can be any atoms - they do not have to be the same or symmetrical.

For example, we can look at nitrite ion: The double bond could be on either side (note – the ion should have brackets and a charge)



If a molecule has a resonance structure, you must indicate both structures using the double headed arrow ($\longleftrightarrow$) to indicate that the molecule can exist in both possible states.

We also looked at CO₂ in class. We know that nature prefers a double bond on both sides since double bonds are lower in energy than a triple bond.



The arrows are just indicating moving those electrons around to go from a single to a double or triple bond.

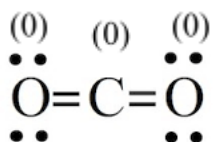
Formal Charge

Formal charge is a useful tool to help determine the best Lewis structure when more than one possible structure exists.

To calculate a formal charge:

$$\text{Formal Charge (FC)} = \text{valence } e^- - \text{associate } e^-$$

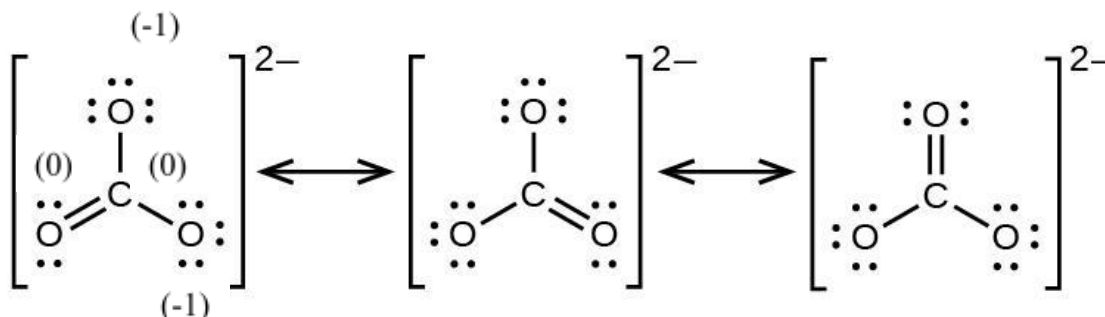
The associated electrons are counted as 1 for each individual electron dot and 1 for each bond. For example, given the structure of the CO₂



Carbon FC = 4 valence e^- - 4 (1 for each bond) = 0 Then we write it on the C with a zero in parenthesis.

FC for O double bonded = 6 valence e^- - 6 associate e^- (1 for each bond and 1 for each dot) = 0

When calculating formal charges on a polyatomic ion, the formal charges should add up to the overall charge of the ion.



For the first structure:

$$\text{FC of C} = 4 - 4 = 0$$

$$\text{O with double bond: } 6 - 6 = 0$$

$$\text{O with single bond: } 6 - 7 = -1$$

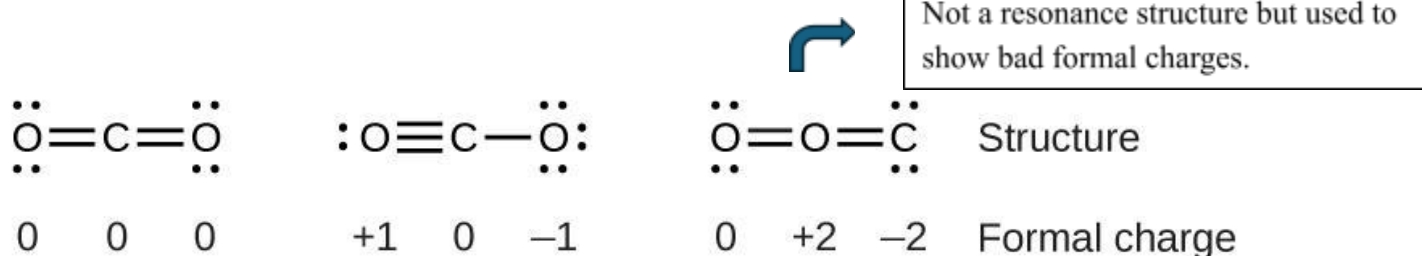
Notice the two -1 charges add up to a -2 for the overall ion. This equals the charge of the ion!

Since formal charges are used to determine the most stable structure in nature, we need to understand what to look for.

Preferred structures have:

- Formal charges of Zero.
- If not zero: the arrangement with the smallest formal charge. (1 versus a 2 or 3)
- Formal charges that are adjacent or of the opposite sign. (adjacent meaning next to each other)
- The negative formal charges on the more electronegative atoms.

Let's look at 3 legitimate Lewis structures for CO_2 and decide which is the most stable.



Looking at the charges, the first option is the most stable because it has the lowest formal charges of all zero – that is ideal. The worst structure is the third option. It has a +2/-2 which are high charges and there is a +2 on the most electronegative oxygen atom. If there are charges – we want a negative charge

on the most electronegative atom. Having a positive charge on an electronegative atom introduces instability.