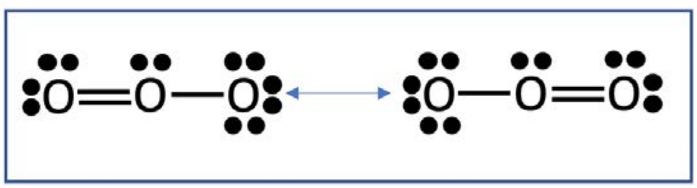
1 Resonance

Often, there are many ways that electrons can be arranged around a molecule. The existence of multiple electronic configurations that are stable leads to *resonance*, which describes the delocalization of electrons in covalently bonded molecules. To be considered resonance structures, molecules must meet the following criteria:

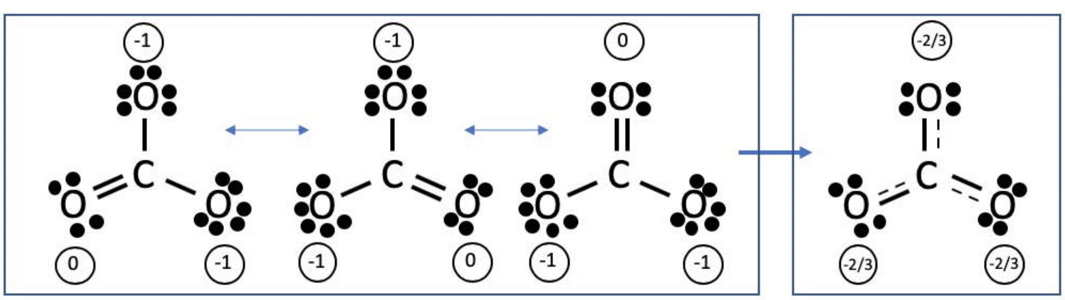
1. Atoms must be in the same orientation relative to each other
2. All resonance structures must have the same number of valence electrons
3. The octet rule must be satisfied, with a few exceptions:
   - Not followed by some elements in periods three and higher, including Cl, Br, I, P, Si
   - Sulfur can have up to 12 e^-
   - Boron can have 6 e^-
4. Formal charge should be on the most electronegative atoms

Example: Draw resonance structures for ozone (O_3) and CO_3^{2-}.

Ozone consists of three oxygen atoms, for a total of 18 valence electrons. These can be equivalently distributed in two ways:



CO_3^{2-} consists of a central carbon atom which brings 4 valence electrons, and four oxygen atoms that each bring 6 electrons, and two additional electrons that yield the additional 2^- charge. The resonance structures can be represented as follows:



These equivalent structures can be combined into one compact picture (shown above on the right) that is an average of the possible structures. All of the resonance structures are equally likely, as they equivalently satisfy the guidelines for stable Lewis structures.

2 Formal charge (again)

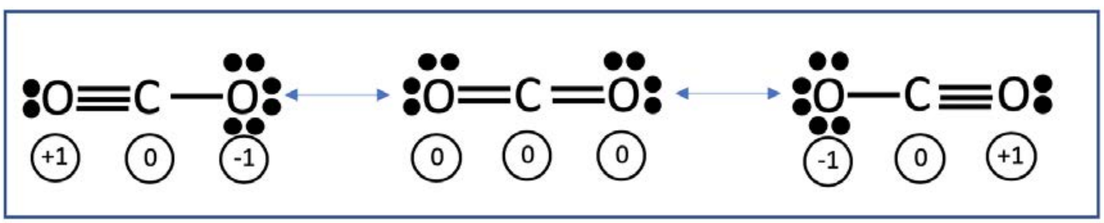
In the CO_3^{2-} example above, the formal charge on each atom is shown in circles. The formal charge only appears on the oxygen, as oxygen is more electronegative than carbon. In the average structure, the formal charge is averaged over all of the oxygen atoms. We can check that we have the most stable resonance structure by evaluating the formal charge on various options. The resonance structure with the lowest formal charge on each atom is the most stable and will occur with higher probability over other resonance structures. As a reminder, formal charge is calculated using

$$\text{Formal Charge} = \#\ \text{valence } e^{-}\text{s} - \left(N + \frac{b}{2}\right)$$

where the number of valence electrons refers to the neutral atom in isolation, N = the number of nonbonding valence electrons and b = the number of valence electrons participating in bonds. Formal charge should be calculated for each atom in the molecule.

Example: Find three resonance structures of CO_2, and determine which is the most stable.

Last recitation, we drew one possible electronic structure of CO_2. Two more are given here:



The formal charge on each atom in each of the three viable resonance structures is shown. Though each resonance structures satisfies the rules of valid Lewis dot diagrams and viable resonance structures, the central structure is the most stable as the formal charge is lowest.