CH 222 Guide to Formal Charges

The **formal charge** for an atom in a molecule or ion is the charge calculated for that atom based on the Lewis structure of the molecule or ion using the following equation:

$$\textbf{Formal Charge} = \textbf{GN} - \textbf{lpe} - {}^{1}/_{2}(\textbf{bpe})$$

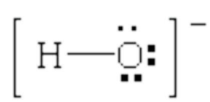
where **GN** = group number for the atom

lpe = number of lone pair electrons on the atom

bpe = number of bonding pair electrons on the atom

- The sum of the formal charges on the atoms in a molecule or ion always equals its net ionic charge.
- Formal charges can be helpful when deciding on the *most likely resonance structure*; the structure with the lowest overall formal charges will be the most likely resonance structure
- Alternatively, the most likely resonance structure will have the lowest absolute value of individual formal charges; i.e. the resonance structure with the lowest summation of the absolute values of *each* formal charge in the molecule or ion will be the most preferred structure

Example: Hydroxide, OH^-, has a net ionic charge of –1 and it has the Lewis structure:

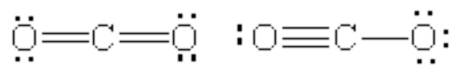


The hydrogen atom in hydroxide has a group number = 1, it has no lone pair electrons, and it has two bonding pair electrons in the single bond. Therefore, the formal charge on the hydrogen atom is: $1 - 0 - {}^{1}/_{2}\,(2) = \mathbf{0}$

The oxygen atom in hydroxide has a group number = 6, it has six lone pair electrons, and it has two bonding pair electrons in the single bond. Therefore, the formal charge on the oxygen atom is: $6 - 6 - {}^{1}/_{2}\,(2) = \mathbf{-1}$

The sum of formal charges is $0 + (-1) = \mathbf{-1}$, which is equal to the net ionic charge of -1.

Example: Carbon dioxide, CO_2, has a net ionic charge of zero. Two possible Lewis structures:



Structure A Structure B

The carbon atom in *both* **A** and **B** has a group number = 4, it has no lone pair electrons, and it has eight bonding pair electrons (in **A**, eight electrons come two double bonds; in **B**, two come from the single bond and six from the triple bond.). Therefore, the formal charge on the carbon atom is: $4 - 0 - {}^1/_2\,(8) = \mathbf{0}$

In structure **A**, *each* oxygen atom has a group number = 6, four lone pair electrons, and four bonding pair electrons in the double bond. Therefore, the formal charge on the oxygen atom is: $6 - 4 - {}^1/_2\,(4) = \mathbf{0}$

In structure **B**, the oxygen atom with the triple bond has a group number = 6, two lone pair electrons, and six bonding pair electrons from the triple bond. Therefore, the formal charge on this oxygen atom is: $6 - 2 - {}^1/_2\,(6) = \mathbf{+1}$

In structure **B**, the oxygen atom with the single bond has a group number = 6, six lone pair electrons, and two bonding pair electrons from the single bond. Therefore, the formal charge on this oxygen atom is: $6 - 6 - {}^1/_2\,(2) = \mathbf{-1}$

Note that the sum of the formal charges in both structures equals the ionic charge:

In **A**, $0 + 0 + 0 = 0$

In **B**, $0 + 1 - 1 = 0$

However, structure **A** is preferred over **B** because **A** has lower formal charges overall. Nature prefers resonance structures with lower formal charges.

The most preferred structure will have the lowest absolute value of individual formal charges:

A: $|\,0\,| + |\,0\,| + |\,0\,| = 0$

B: $|\,0\,| + |\,1\,| + |\,-1\,| = 2$