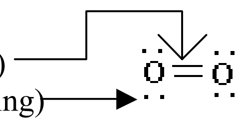
Formal Charge and Lewis Structure

To start with, when the Lewis structure is written, total number of valence electrons is distributed according to certain rules, such as, octet, duet, etc. When you do that, some atoms gain electrons and some atoms loose electrons compared to their valence electrons. To know which atom loses the electrons and which atoms gain the electrons, you need to compute the formal charge.

Thus, the **formal charge** is defined as the electrical charge that is the difference between the valence electrons in an isolated atom and the number of electrons assigned to that atom in a Lewis structure. That means, you have to compare electrons around an atom in Lewis structure with those in isolated atom (valence electrons).

The Lewis structure involves two kinds of electrons around an atom:

Bonding electrons (electrons engaged in bonding)
Nonbonding electrons (electrons other than bonding)



IMPORTANT: You must understand how to identify these two kinds of electrons before you continue.

The formal charge for each atom is calculated using the following formula:

Formal charge on an atom = [Total number of valence electrons]
– [Total number nonbonding electrons]
– 1/2 [Total number of bonding electrons]
= VE – NBE – 1/2 BE (this is my notation)

Since the bonding electrons are shared between two atoms, we must divide the bonding electrons equally between two atoms, and hence the 1/2 factor in the above formula.

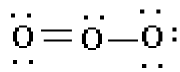
The calculated formal charge using the above equation can be positive (+) to mean excess electrons (VE > [NBE+1/2 NE]) or negative (-) to mean gain of electrons (VE < [NBE+1/2 NE] or zero mean nothing is gained or no excess electrons (VE = [NBE+1/2NE]). Keep in mind that the following rules apply when you calculate the formal change.

- For neutral molecule, the sum of formal charges must add up to zero.
- For positive ion (cation), the sum of formal charges must add up to the positive charge on the cation.
- For negative ion (anion), the sum of formal charges must add up to the negative charge on an anion.

Examples

1. Neutral molecule

Ozone (allotropic form of oxygen), is a triatomic form of oxygen with the following Lewis structure:



The formal charges are calculated as follows.

- The end left O atom in O=O bond: This atom has 6 valence electrons (VE), 4 bonding electrons (BE), and 4 nonbonding electrons (NBE), then

  Formal charge = VE – NBE – 1/2 BE
  = 6 – 4 – 1/2 x 4 = 0

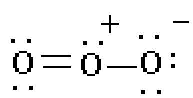
- The central O atom: This atom has 6 valence electrons, 2 nonbonding electrons, and 6 bonding electrons, then

  Formal charge = 6 – 2 – 1/2 x 6 = +1

- The end right O atom in O-O bond: This atom has 6 valence electrons, 6 nonbonding electrons, and 2 bonding electrons, then

  Formal charge = 6 – 6 – 1/2 x 2 = -1

Now the Lewis structure with formal charges is written as,



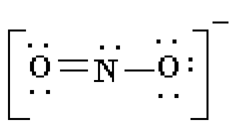
Note that the total charge is zero [(+) + (-) = 0] as should be for neutral atom and the zero formal charge usually is not indicated on an atom.

IMPORTANT: You must calculate the formal charge for each atom in a molecule.

2. Negative ion (anion)

Consider the nitrite ion (NO_2^-).

The Lewis structure for this ion is



The formal charges are calculated as follows.

- The end left O atom in O=N bond: This atom has 6 valence electrons, 4 nonbonding electrons, and 4 bonding electrons, then

  Formal charge = 6 – 4 – 1/2 x 4 = 0

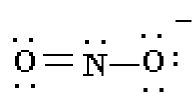
- The central N atom: This atom has 5 valence electrons, 2 nonbonding electrons, and 6 bonding electrons.

  Formal charge = 5 – 2 – 1/2 x 6 = 0

- The end right O in N-O bond: This atom has 6 valence electrons, 6 nonbonding electrons, and 2 bonding electrons, then

  Formal charge = 6 – 6 – 1/2 x 2 = -1

Now the Lewis structure with formal charges is

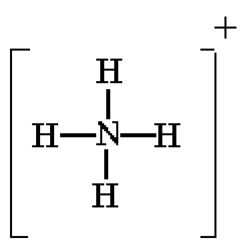


NOTE: The sum of the formal charges is -1, which is equal to the charge on the nitrite ion.

3. The positive ion (cation)

Consider the ammonium ion (NH_4^+).

The Lewis structure for this ion is



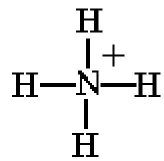
- The central N atom: This atom has 5 valence electrons, zero nonbonding electrons, and 8 bonding electrons.

  Formal charge = 5 – 0 – 1/2 x 8 = +1

- Terminal H atoms: All these atoms are equivalent. The H atom has 1 valence electron, zero nonbonding electrons, and 2 bonding electrons. Then,

  Formal charge = 1 – 0 – 1/2 x 2 = 0

The Lewis structure with formal charges is



NOTE: The sum of the formal charges (+) is the same as the charge on the ammonium ion.