How to Determine Formal Charges

What Are Formal Charges?

Formal charges are charges we assign to each atom in a Lewis structure. This is not to be confused with the net charge of an ion. For example, the nitrate ion, NO₃⁻ has a net charge of −1. The N atom has a formal charge of +1 and each oxygen atom that is singly-bonded to N has a formal charge of −1.

Why Do We Need Formal Charges?

Often it is useful to know exactly which part of the molecule that is charged. If you look at the formula of the nitrate ion, NO₃⁻, you only know that the net charge is −1 but you don’t know where it is. The formula NO₃⁻ is not implying that the −1 is on the O.

In addition, the formal charges give us a means to determine whether a particular structure is reasonable; or, if you have several resonance structures, the formal charges will help you determine which resonance structure is preferred over the others. For example, you would not like to have a structure with a positive formal charge on a highly electronegative element (such as oxygen). You would also avoid writing a Lewis structure with a lot of formal charges (although in some cases it cannot be avoided). Often it is preferred to violate the Octet Rule in order to achieve a zero formal charge on an atom.

Rules for Assigning Formal Charges

First you must have a Lewis structure that shows all the lone pairs (nonbonding electrons). This tutorial is not meant to show you how to draw Lewis structures, but how to assign formal charges, after you have one to look at. [See separate tutorial on how to write Lewis Structures.]

1. Examine each atom in the Lewis structure, one at a time.
2. Count both electrons in a lone pair (nonbonding electrons) and one electron per bond.
3. Compare this number with the Group # (from the periodic table), which tells you how many the atom is supposed to have.
4. The Group # tells you how many electrons a neutral atom would have. So, if you have one more electron than the Group # indicates, the atom has a formal charge of −1. If you have two more electrons, the charge is −2, and so forth.
5. If you have one less electron than the Group # indicates, the atom has a charge of +1. If you have two less electrons, the charge is +2, and so forth.
6. If you prefer to memorize an equation, it would be

\[
\text{Formal Charge} = \text{Group Number} - (\text{number of nonbonding electrons} + \text{number of bonds})
\]

Personally I would suggest you use logic rather than memorizing an equation that you can easily forget. If you use logic, chances are much better that you can always figure it out even when your memory fails you.
Example 1

Let us return to our example of the nitrate ion.

\[
\begin{array}{c}
\text{O} \\
\text{N} \\
\text{O}
\end{array}
\]

For the O with the double bond, we are counting 6 electrons for it (4 nonbonding electrons and 2 bonding electrons (one per bond). Since O is in Group VIA, that’s how many electrons it should have, so the charge for that O is zero (which is usually not shown).

For either of the O atoms with a single bond, we are counting 7 electrons (6 nonbonding electrons and one bonding electron). That’s one more than 6, so those O atoms have a charge of $-1$ each.

For N, we are counting 4 electrons (4 bonding electrons, no nonbonding electrons). Since N is in Group VA, we have one less electron than N should have, and so it has a $+1$ charge.

As a check, your formal charges should add up to the charge of the atom ($-1$ for nitrate).

You might have learned that it is not good to leave a positive charge on the central atom and that you should consider bringing in one of the lone pairs from a neighboring O as shown below:

\[
\begin{array}{c}
\text{O} \\
\text{O} \\
\text{N}
\end{array}
\]

This might seem a more reasonable structure as it would minimize the number of formal charges. HOWEVER, NITROGEN CANNOT VIOLATE THE OCTET RULE WITH GOING BEYOND 8 ELECTRONS!

We count both electrons in a bond when checking on the Octet Rule, and in the structure shown above, N would have 10 electrons. Only elements beyond atomic number 10 (Ne) can exceed the Octet Rule. Atoms with atomic numbers less than 10 do not have d-orbitals to accommodate the extra electrons.

Example 2

\[
\begin{array}{c}
\text{H} \\
\text{H} \\
\text{N} \\
\text{H}
\end{array}
\]

What is the formal charge on the H atoms?
What is the formal charge on the N?

We count one electron for each H, and that’s how many it should have, so the H atoms are all neutral. We count 4 bonding electrons for N, which should have 5, so the formal charge is $+1$.

The net charge is $+1$ which checks out with the charge of the ammonium ion ($\text{NH}_4^+$).

Here are some questions for you to practice on. I recommend you copy the structure onto a piece of paper and work out the formal charges before you look at the answers provided.
PRACTICE QUESTIONS

Determine the formal charges in each of the following:
(Note: The structures shown are not meant to be the “correct” Lewis structures. After you have finished assigning formal charges and you examine the answers provided, you will that I have made comments on the once that are not likely to exist based on the formal charges.)

1. ClO₃⁻  
   :O─Cl─O:
   :O:

2. CHO₂⁻  
   :O─H─C─O:
   :O:

3. CO₂  
   :O─C≡O:
   :O:

4. C₂H₃Cl  
   :Cl─C─C─H
   :H

Before looking at the answers provided below, write down your answers on a piece of paper.
Ans to #1 (ClO$_3$\(^{-}\))

\[
\begin{align*}
\text{Cl} & \quad \text{O} \\
\text{O} & \quad \text{O} \\
\text{O} & \quad \text{2+} \\
\text{O} & \\
\text{O} & \\
\end{align*}
\]

Note the net charge is \(-1\), which coincides with the charge of the chlorate ion.

Note that this is a case where you should violate the Octet Rule in order to give Cl an neutral formal charge by bringing in a lone pair each from two of the O atoms to give you the structures below. Cl has an atomic number greater than 10 and therefore can exceed the Octet Rule:

\[
\begin{align*}
\text{:O=Cl=O:} & \quad \text{\textarrow{}\textarrow{}} \quad \text{:O=\text{\textbullet{}}Cl=O:} & \quad \text{\textarrow{}\textarrow{}} \quad \text{:O=Cl\text{\textbullet{}}O:} \\
\text{:O:\text{\textbullet{}}} & & & & & & & & & & \text{O:} \\
\end{align*}
\]

Ans to #2 (CHO$_2$\(^{-}\))

\[
\begin{align*}
\text{O} & \quad \text{H} \\
\text{H} & \quad \text{C} \\
\text{O} & \\
\end{align*}
\]

Ans to #3 (CO$_2$)

(This is one of the possible resonance structures for CO$_2$, but it is not a major contributor because it places a positive charge on O which is a highly electronegative element. This is an example that shows how formal charges help you decide whether a particular resonance structure should be considered.)

\[
\begin{align*}
\text{O} & \quad \text{\textbullet{}} \\
\text{C} & \quad \text{=O} \\
\end{align*}
\]

Ans. to #4 (C$_2$H$_3$Cl)

\[
\begin{align*}
\text{Cl} & \quad \text{C} \\
\text{H} & \quad \text{C} \\
\text{H} & \\
\end{align*}
\]

This is also not a major contributor, especially since there is another resonance form to this that does not contain any formal charges.

END OF TUTORIAL