Formal Charge in Lewis Structures

Assigning electrons to nuclei

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A Useful Tool

Formal charge is a way of looking at how electrons are distributed in a molecule or polyatomic ion. It can be used to help assess a structure as well as predict reactivity or other properties.

For anyone who will be taking organic chemistry, formal charge will be a very helpful concept to have in your toolbox.

Calculating Formal Charge

Formal Charge treats electrons as if all bonds are purely covalent. The steps are:

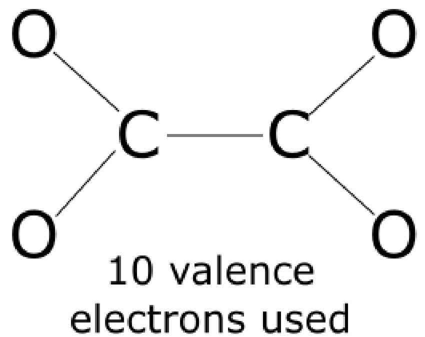
1. Draw a Lewis Structure
2. For electron pairs in bonds, “assign” one electron to the element on each end of the bond. (“split the bonds”)
3. For lone pairs or unpaired electrons, assign them to the atom upon which they are drawn
4. Compare the number of “assigned” electrons to the number of electrons in the neutral atom

This is easier to see with an example…

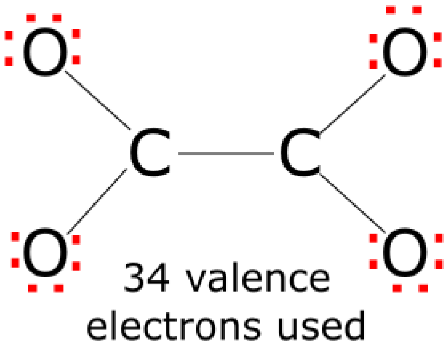
Oxalate Ion – Formal Charge

First step: Draw a Lewis Structure; Oxalate Ion = $C_2O_4^{-2}$

1. Count valence electrons. (2x4 for carbon) + (4x6 for oxygen) + (2 extra for the "-2" charge) = 34 valence electrons
2. Draw a skeleton with all single bonds



3. Fill octets of peripheral atoms (oxygens in this case)



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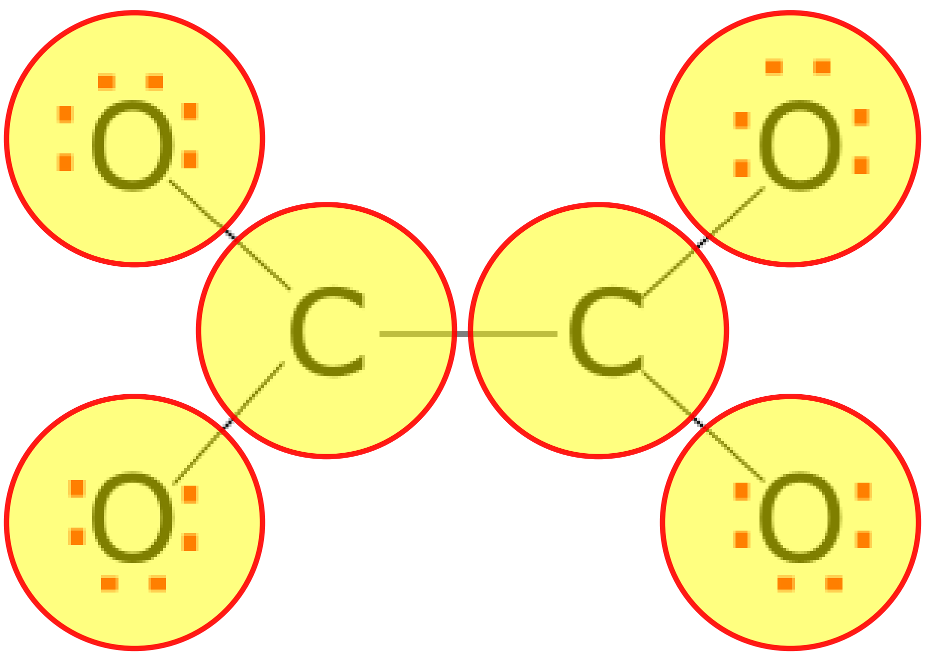
Assigning Electrons

Now we can draw some circles to assign electrons to each nucleus (atom).

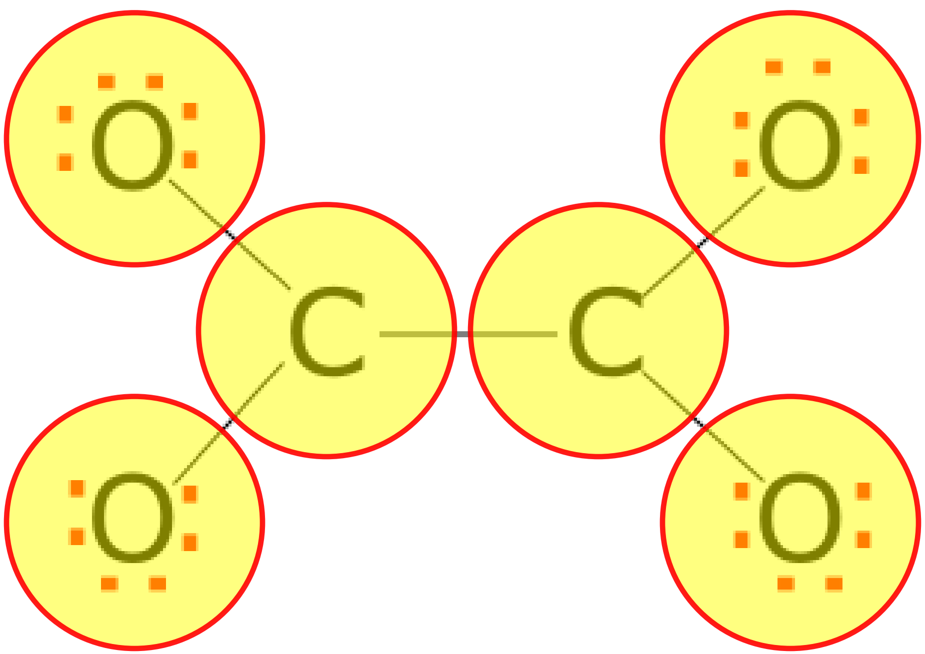


Each oxygen is assigned 6 electrons from the 3 lone pairs and 1 electron from the bond.
7 electrons assigned.

Each carbon is assigned 1 electron from each of the 3 bonds.
3 electrons assigned

Formal Charges

Compare the assigned electrons to the electrons in the neutral atom.



For oxygen:

Assigned e^{-}s = 7

Neutral e^{-}s = 6

Formal charge = -1

{1 more electron assigned than in neutral}

For carbon:

Assigned e^{-}s = 3

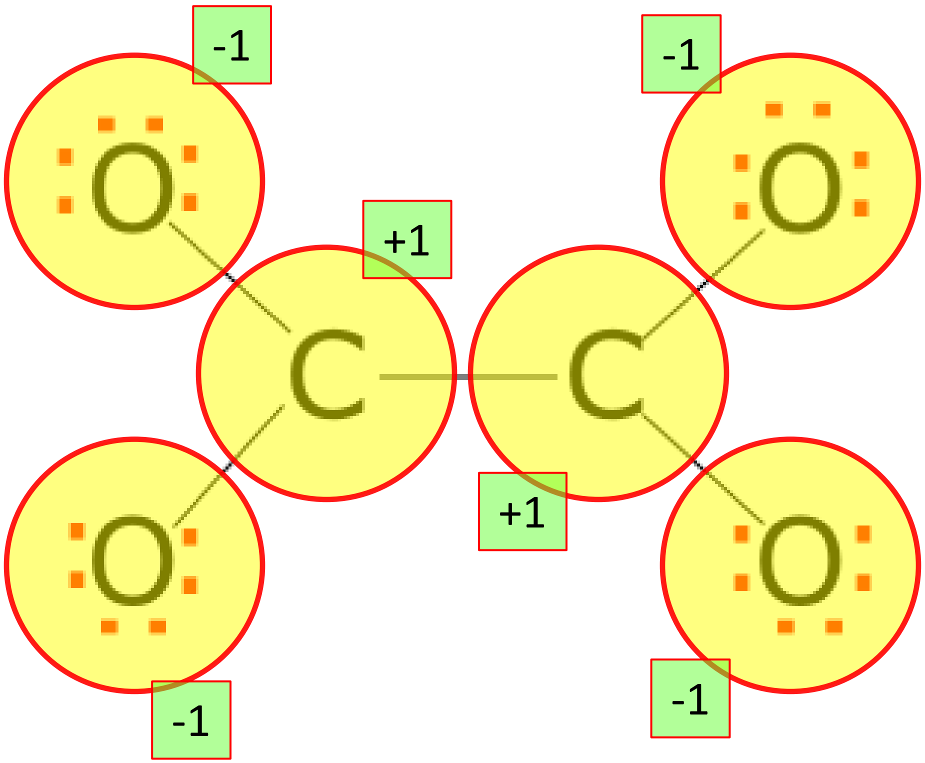
Neutral e^{-}s = 4

Formal charge = +1

{1 less electron assigned than in neutral}

Check your work!

The sum of the formal charges must equal the charge of the ion (or be zero for molecules)

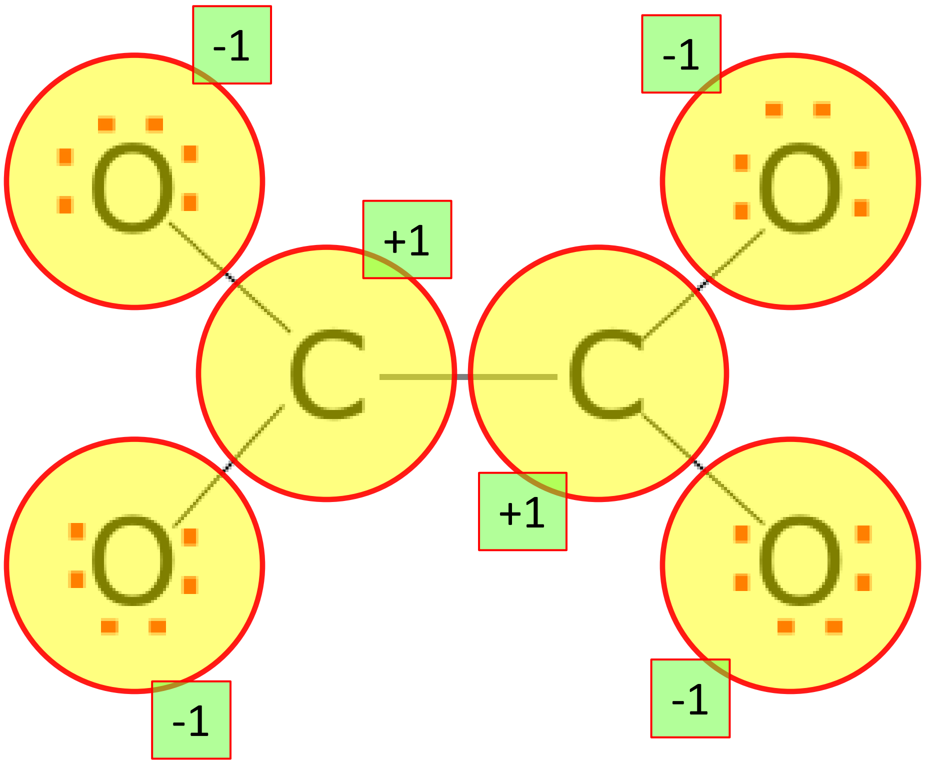


$4(-1) + 2(+1) = \mathbf{-2}$

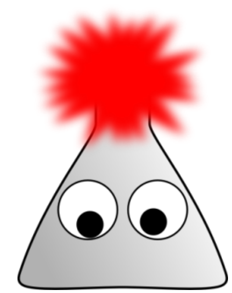
This means we have accounted for all of the electrons in the structure.

“Good” Lewis Structure?

A “good” Lewis Structure tends to minimize the formal charge distribution (as possible).



This Lewis Structure has formal charge scattered *everywhere*. The carbons also don’t have an “octet”.



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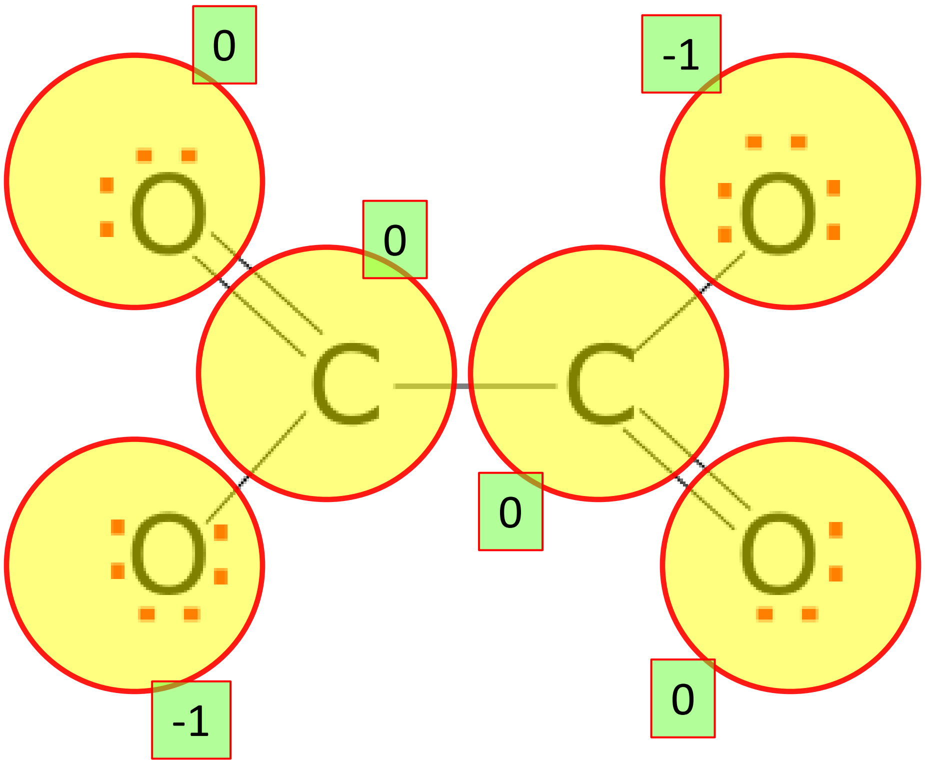
A Better Lewis Structure?

Sharing some of the oxygen lone pairs with the carbon to form double bonds helps.



The formal charge distribution has been minimized.

The carbons each have an "octet".

A final note…

Notice that the sum of the formal charges is still -2. We did *not* add or subtract electrons when we made the double bonds, we just moved electrons around.