Oxidation Numbers in Lewis Structures

Assigning electrons to nuclei

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Another Useful Tool

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

There are a number of ways to determine oxidation numbers, this is a *structural* way.

Calculating Oxidation Numbers

Oxidation Numbers treat electrons as if all bonds are purely ionic. The steps are:

1. Draw a Lewis Structure
2. For electron pairs in bonds, “assign” all bonding electrons to the more electronegative element. For bonds between elements of the same electronegativity, assign one electron to each atom
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…

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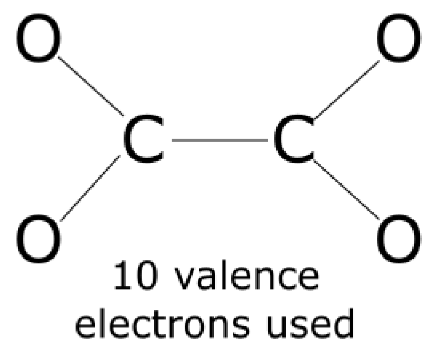
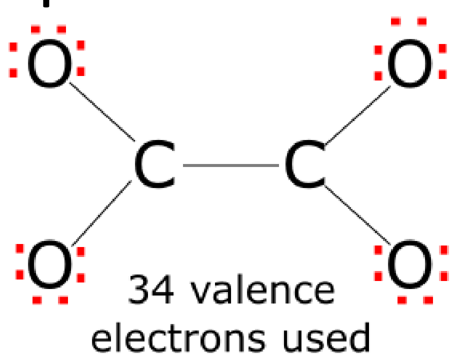
Oxalate Ion – Oxidation Number

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

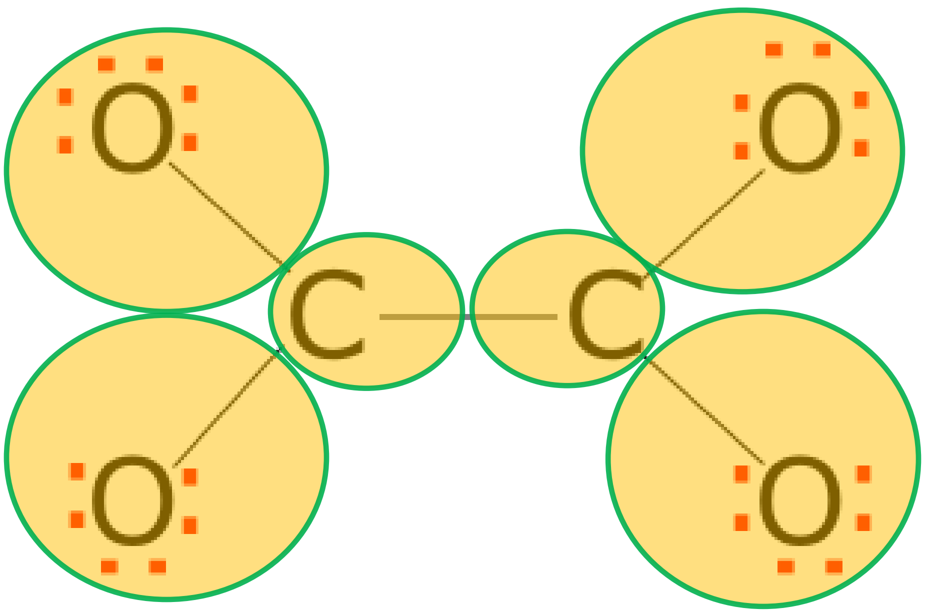


3. Fill octets of peripheral atoms (oxygens in this case)



Assigning Electrons

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

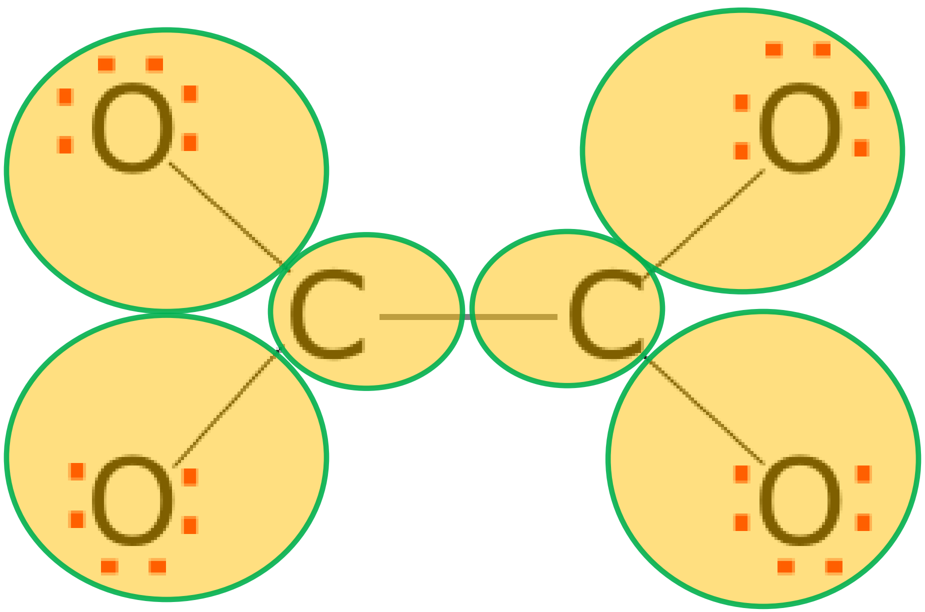


Each oxygen is assigned 6 electrons from the 3 lone pairs and 2 electron from the bond.
{O more electronegative than C}
8 electrons assigned.

Each carbon is assigned 1 electron from the C-C bond.
1 electrons assigned

Oxidation Numbers

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



For oxygen:

Assigned e^-s = 8

Neutral e^-s = 6

Oxidation Number = -2

{2 more electron assigned than in neutral}

For carbon:

Assigned e^-s = 1

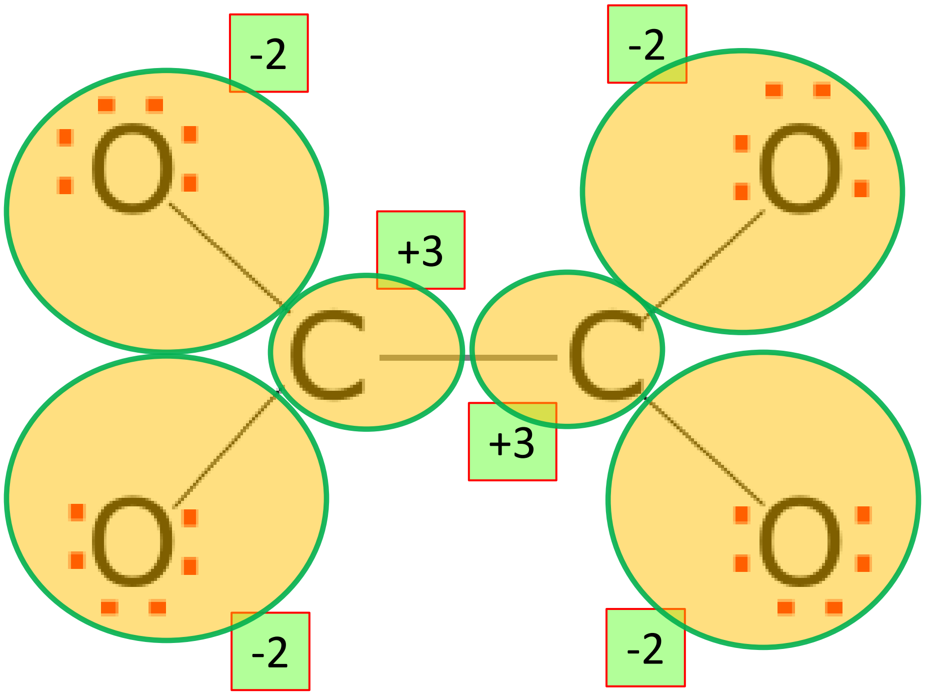
Neutral e^-s = 4

Formal charge = +3

{3 less electron assigned than in neutral}

Check your work!

The sum of the oxidation numbers must equal the charge of the ion (or zero for molecules)



$4(-2) + 2(+3) = \mathbf{-2}$

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

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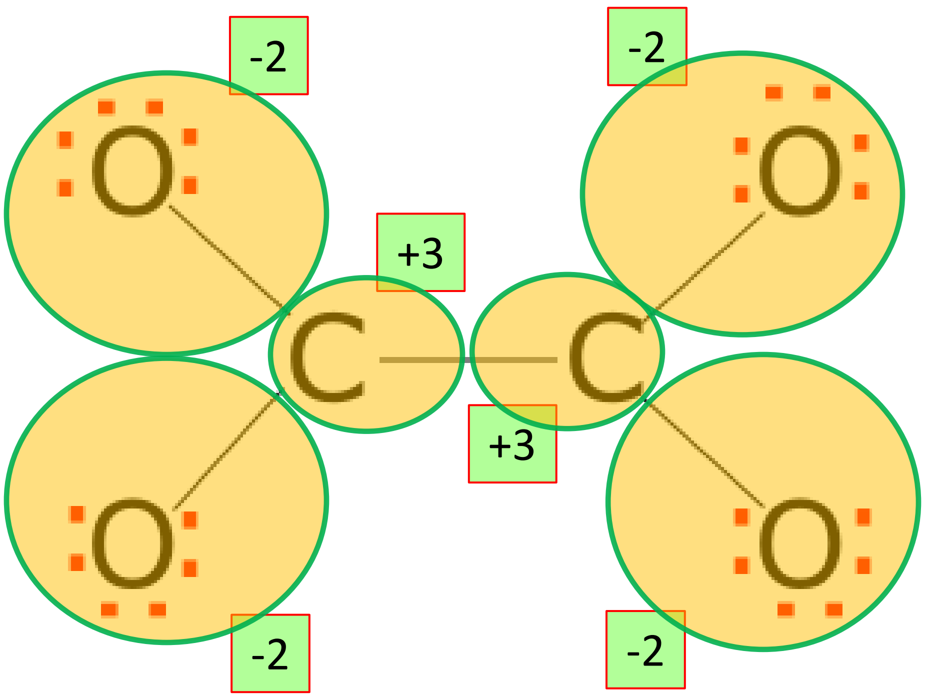
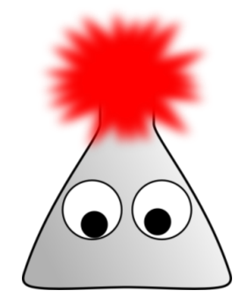
“Good” Lewis Structure?

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

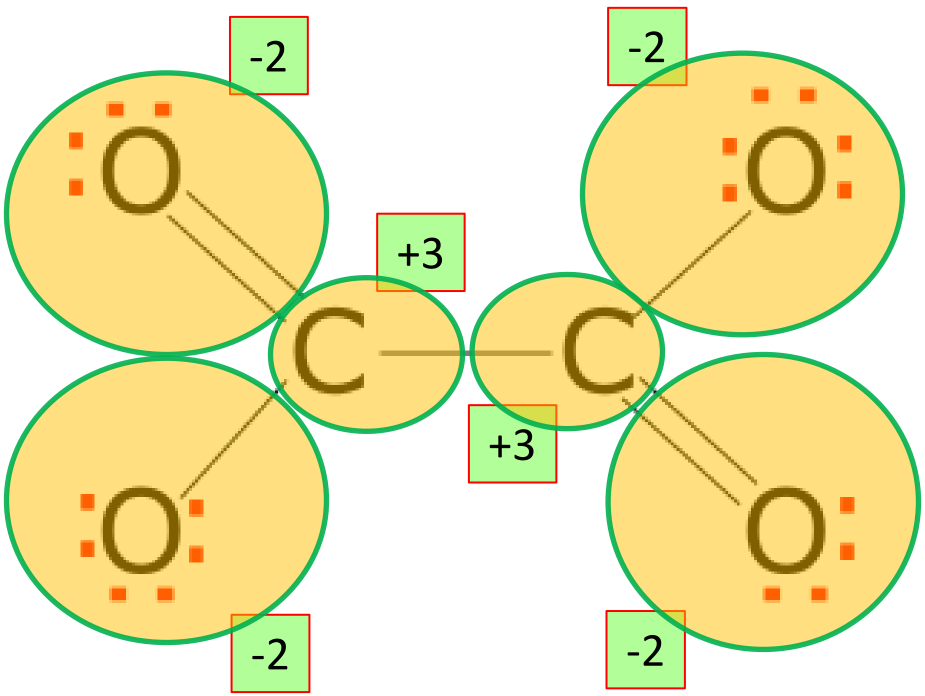


This Lewis Structure has oxidation numbers scattered *everywhere*. The carbons also don’t have an “octet”.



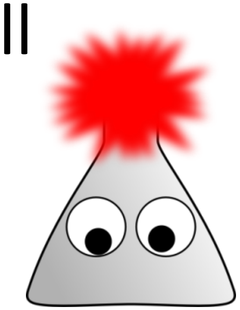
No change!

Forming double bonds has no effect on the oxidation numbers in this case!



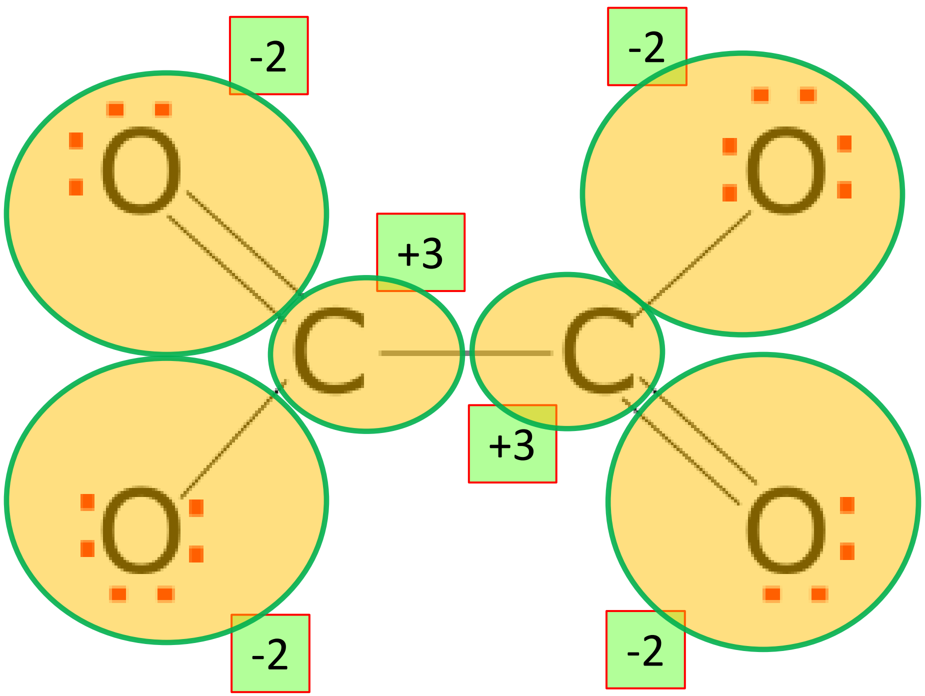
Because oxidation numbers treat all bonds as if they are purely ionic, they tell us more about the individual atoms than the molecule as a whole.

The carbon octets still make this a better Lewis Structure.



A final note…

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



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