

About Oxidation States

Atoms tend to participate in bonding in such a manner that their electronic configuration becomes similar to that of the nearest inert gas.

Why?

Because the electronic configuration of an inert gas is particularly stable

In other words, an atom involved in bonding tends to acquire or lose the smallest possible number of electrons that will cause its electronic configuration to become inert gas – like.

Why the smallest possible number of electrons?

Because acquiring and – especially – losing electrons costs energy.

Example:

H								He
Li	Be		B	C	N	O	F	Ne
Na	Mg		Al	Si	P	S	Cl	Ar

Li tends to participate in bonding by losing 1 electron, so that its electronic configuration becomes similar to that of He, rather than acquiring 7 electrons and become Ne-like

F tends to participate in bonding by acquiring 1 electron, so that its electronic configuration becomes similar to that of Ne, rather than losing 7 electrons and becoming He-like

Mg tends to participate in bonding by losing 2 electrons, so that its electronic configuration becomes similar to that of Ne.

Oxygen tends to participate in bonding by acquiring 2 electrons, so that its electronic configuration becomes similar to that of Ne.

The oxidation state of an atom is a measure of how close its electronic configuration might be to that of an inert gas.

An atom involved in bonding loses or gains electrons (in a formal sense) by establishing bonds to atoms of higher / lower electronegativity.

Consider a C—O bond. This interaction is the result of C and O each contributing 1 electron to the bond. Because O is more electronegative than C, the O atom attracts the σ electron pair that we call "bond" more strongly than the C atom. The σ electron pair will be distorted toward the oxygen, i.e., the two electrons will reside preferentially in

proximity of the O atom. Thus, bonding has caused the C atom to formally lose an electron (to the O), and the O atom to formally acquire an electron (from the C).

We express this fact by saying that the oxidation state of the C atom has increased by 1 unit (= it has become +1) and that the oxidation state of the O atom has decreased by 1 unit (= it has become - 1) as a result of bonding.

Because of this, the C atom has moved closer to He, the O atom to Ne, in terms of electron configuration.

The oxidation state of an atom in a molecule is the sum of all such effects resulting from bonding, plus the formal charge possibly present on the atom.

Example 1: the oxidation state of C in CH₃Cl

Carbon forms 1 bond to chlorine, 3 bonds to H, and it has no formal charge. Cl is more electronegative than C, so carbon loses 1 electron to Cl as a result of the C-Cl bond. H is less electronegative than C, so carbon gains 3 X 1 electrons as a result of the C-H bonds.

Now we can calculate the oxidation state of C:

<i>bonding:</i>	C-Cl	+1
	C-H	-1
	C-H	-1
	C-H	-1
<i>formal charge:</i>		0
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Oxidation state:		-2

Example 2: the oxidation state of the starred C in *CH₃-CH₃

This molecule presents a C-C bond. Because the 2 C atoms have the same electronegativity, there is neither gain nor loss of electrons as a result of this bonding interaction. H is less electronegative than C, so carbon gains 3 X 1 electrons as a result of the C-H bonds.

<i>bonding:</i>	C-C	0
	C-H	-1
	C-H	-1
	C-H	-1
<i>formal charge:</i>		0
=====		
Oxidation state:		-3

Example 3: the oxidation state of N in $^{(+)}\text{N}(\text{CH}_3)_4$

N is more electronegative than C and it has a formal + charge in this molecule:

<i>bonding:</i>	N-C	-1
	N-C	-1
	N-C	-1
	N-C	-1
<i>formal charge:</i>		+1

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Oxidation state: -3

Example 4: the oxidation state of the starred C in $\text{CH}_3\text{-}^*\text{CH}^{(-)}\text{-CH}_3$

The C in question has a formal (-) charge:

<i>bonding:</i>	C-C	0
	C-C	0
	C-H	-1
<i>formal charge:</i>		-1

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Oxidation state: -2

Example 5: the oxidation state of C in CH_2Cl_2

The C in question has a formal (-) charge:

<i>bonding:</i>	C-Cl	+1
	C-Cl	+1
	C-H	-1
	C-H	-1
<i>formal charge:</i>		0

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Oxidation state: 0

Example 6: the oxidation state of C in $^{(-)}\text{C}\equiv\text{O}^{(+)}$

The C in question has a formal (-) charge and it forms 3 bonds to O:

<i>bonding:</i>	C-O	+1
	C-O	+1
	C-O	+1
<i>formal charge:</i>		-1

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Oxidation state: +2

Example 7: the oxidation state of the starred C in CH₃-*COOH

<i>bonding:</i>	C-O	+1
	C-O	+1
	C-O	+1
	C-C	0
<i>formal charge:</i>		0

Oxidation state:	+3
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Example 8: the oxidation state of C in O=C=O

<i>bonding:</i>	C-O	+1
	C-O	+1
	C-O	+1
	C-O	+1
<i>formal charge:</i>		0

Oxidation state:	+4
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Atoms tend to participate in bonding by acquiring particular oxidation states that reflect a favorable electronic configuration. An atom present within a molecule at an unfavorable oxidation state will tend to advance to a more favorable oxidation state by gaining/losing electrons as appropriate. Therefore, oxidation states are important measures of the reactivity of a given atom, and that's why we must be able to recognize the oxidation state of an atom at a glance.

Furthermore, many organic reactions proceed so that no change occurs in the oxidation state of atoms, whereas other reactions do involve changes in such oxidation states. A reaction that involves a change in oxidation is called a *redox* reaction. Redox processes require the use of appropriate oxidants or reductants. If we want to achieve a generic organic transformation, it is obviously essential to know whether redox chemistry is involved, i.e., whether oxidants / reductants will have to be employed. That's one additional reason that oxidation states are so important in organic chemistry.