

Chemical Bonding Terms



To calculate the oxidation number of elements in organic molecules using formal charges and Lewis structures, follow these steps:

General Rules for Assigning Oxidation Numbers:

1. **Oxidation number of atoms in their elemental form** (e.g., O₂, N₂, H₂) is zero.
2. **Oxidation number of hydrogen** is generally +1 (except in metal hydrides, where it is -1).
3. **Oxidation number of oxygen** is generally -2 (except in peroxides, where it is -1).
4. The sum of oxidation numbers in a neutral molecule is zero, and in an ion, it equals the charge of the ion.
5. For organic molecules, assign electrons in bonds to the more electronegative element, and then use formal charge balancing.

Steps:

1. **Draw the Lewis structure** of the molecule.
2. **Assign electrons** in bonds to the more electronegative atom.
3. **Calculate oxidation number** using the difference between the number of valence electrons an atom has in its free state and the number assigned to it in the molecule.

Example Calculations:

1. Methane (CH₄)

- Lewis structure:

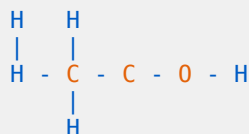


- Hydrogen is less electronegative than carbon, so each C-H bond assigns both bonding electrons to carbon.
- **Oxidation numbers:**
 - Carbon: 4 bonds to less electronegative hydrogen → 4 electrons assigned to C.
 - Oxidation number of carbon = 4 (valence electrons) - 8 (assigned electrons) = -4
 - Hydrogen: Each H has 1 bond to more electronegative C → 0 electrons assigned to H.
 - Oxidation number of hydrogen = 1 (valence electron) - 0 (assigned electrons) = +1

2. Ethanol (C₂H₅OH)

- Lewis structure:

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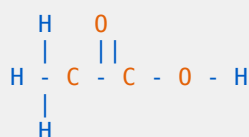


- For **C1** (the first carbon):
 - Bonds to three hydrogens (C-H), so all electrons are assigned to C.
 - Bond to C2: Both C atoms share the electrons equally.
 - Oxidation number of C1 = 4 (valence electrons) - 7 (assigned electrons) = -3
- For **C2** (the second carbon):
 - Bonds to two hydrogens and one oxygen (more electronegative), so assign electrons accordingly.
 - Oxidation number of C2 = 4 (valence electrons) - 5 (assigned electrons) = -1
- For **Oxygen**:
 - Bonds to C2 and hydrogen. Oxygen is more electronegative, so assign both bonding electrons to O.
 - Oxidation number of O = 6 (valence electrons) - 8 (assigned electrons) = -2
- For **Hydrogen**:
 - Oxidation number of each hydrogen = +1 (same as in methane).

3. Acetic Acid (CH₃COOH)

- Lewis structure:

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- For the **CH₃ group**:
 - Carbon has 3 C-H bonds and 1 C-C bond.
 - Oxidation number of C in CH₃ = -3 (similar to methane).
- For the **COOH group**:
 - **C in COOH** (C=O, C-OH): This carbon is attached to an oxygen atom via a double bond and another oxygen atom via a single bond.
 - Oxidation number of carbon = 4 (valence electrons) - 2 (assigned electrons) = +2.
- **Oxygen in OH**: Bonded to hydrogen and carbon, more electronegative, so assign all electrons.
 - Oxidation number = -2.
- **Oxygen in C=O**: Double bond to carbon.
 - Oxidation number = -2.
- **Hydrogen** in the molecule: Oxidation number = +1.

These calculations show how to assign oxidation numbers to elements in organic molecules based on formal charges and Lewis structures.