Introduction to Organic Chemistry | Part [A]

STRUCTURAL FORMULAE

Section - 1

We have already discussed that carbon has tetravalency and the formation of covalent bonds by it is explained in terms of its electronic configuration and the hybridization of s and p orbitals. It may be recalled that formation and shapes of molecules like Methane (C_4H_4), Ethene (C_2H_4), and Ethyne (C_2H_2) were explained in the terms of sp^3 , sp^2 , and sp hybridization of the respective carbon atoms.

Organic chemists use a variety of ways to represent structural formulae of an organic compound. The most common types of representations are shown below.

Dot Structure (Lewis Structure)

This shows all the valence electrons. For example, given below is the dot structure of n-propyl alcohol.

Writing dot structure is tedious and time consuming. The other representations are more convenient and are, therefore, more often used.

Dash Structural Formula

Here, the pair of two electrons forming the covalent bond is represented by a dash. A single dash represents a single bond, double dash is used for double bond and a triple dash represents a triple bond. The lone pair of electrons on hetero-atoms like oxygen, nitrogen, sulphur, halogens, etc. may or may not be shown. Given below is the dash structure of n-propyl n-propyl alcohol.

Condensed Structural Formulae

Condensed structural formulae are easier to write than dash formulae and, when we become familiar with them, they will impart all the information that is contained in the dash structure. In the condensed formula, all the atoms bonded to a carbon atom are written after 'C' in the same line but their bonds are shown. Identical group are omitted by indicating their number as a subscript. The atoms or groups other than hydrogen are written after the hydrogen atom. (in brackets) Given below are the condensed formulae for n-propyl alcohol and isopropyl alcohol.

$$CH_3(CH_2)_2OH$$
 n -Propyl alcohol $CH_3CH(OH)CH_3$ Isopropyl alcohol $CH_3(CH_2)_4CH_3$ n - Hexane

Note: The carbon atoms in organic compounds may also be arranged in rings (Cyclic compounds). For example: cyclopropane, whose structural formula is given alongside.

Bond-Line Formula

A very simplified formula called Bond-line formula can also be used to represent structures of organic compounds. In this representation, the C and H atoms are not shown; the chain of carbon atoms is represented by a zig-zag line. Each intersection of 2 or more lines (junction) and the end of a line represents a carbon atom. Hetero-atoms (other than carbon and hydrogen) or functional groups are specifically written. Hydrogen atoms necessary to fulfil the valence of carbon atoms are assumed to be present.

Bond line formulas are very frequently used for cyclic compounds.

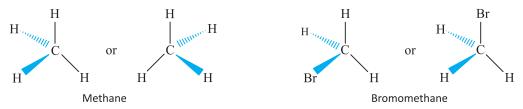
Condensed formula	Bond line formula
CH ₃ CH ₂ CH ₃	
CH ₃ CH ₂ CH ₂ OH	OH
CH ₃ CH(OH)CH ₃	OH
CH_2 CH_2 CH_2	

Multiple bonds are also included in bond-line formula For example:

Condensed formula	Bond line formula
	1 3 4 5
$^{1}_{HC} = ^{2}_{C} - ^{3}_{CH_{2}CH(OH)CH_{3}}^{4}$	2 3 4 5 OH

Three - Dimensional Representation

None of the formulae that we have described so far conveys any information about how the atoms of a molecule are arranged in space. There are several ways to represent the three dimensional structure of the organic molecule on paper. For example: by using a solid and dashed wedge formula, the three dimensional image of a molecule from a two dimensional picture can be perceived. In this representation, bonds that project upwards out of the plane of the paper are indicated by a solid wedge (), those that lie behind the plane are indicated with a dashed wedge (), and those bonds that lie in the plane of the paper are indicated by a line (). Wedges are shown in such a way that the broad end of the wedge is towards the observer. Generally, we only use three-dimensional formulae when it is necessary to convey information about the shape of the molecule.



Wedge and Dash Representation

CLASSIFICATION OF ORGANIC COMPOUNDS

Section - 2

Based upon the nature of carbon atom skeleton, the organic compounds have been classified into two categories: Acyclic or Open Chain and Cyclic or Closed chain.

