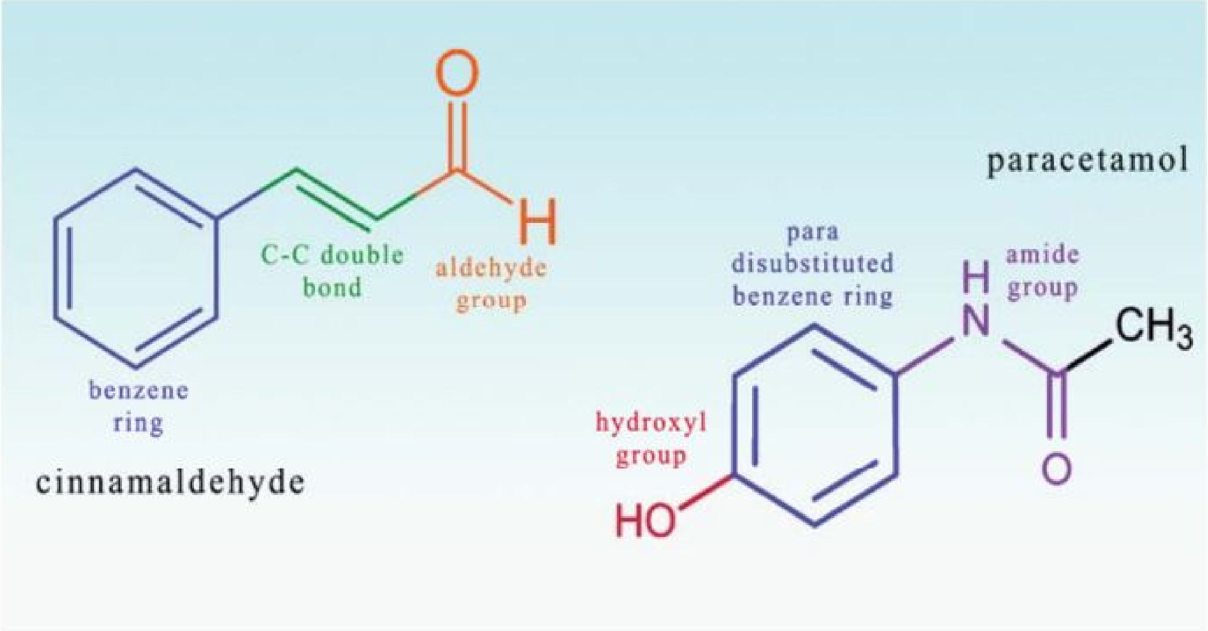


1. Basic Concepts of Organic Chemistry

Content

Introduction

Organic Chemistry is the chemistry of compounds of carbon. In these compounds, carbon atoms form the skeleton or backbone of the molecule. In addition to carbon, organic compounds usually contain hydrogen. Oxygen, nitrogen, sulphur, phosphorus and halogens are also found in certain organic compounds. These compounds can be natural or synthetic. Organic compounds form an essential component of all living organisms and play a central role in metabolic processes. Organic compounds also form an essential component in many of the materials that are essential for our daily life such as food, plastic items, textiles, cosmetics and medicines. The variety and number of compounds formed by carbon is very large compared to the compounds formed by other elements in the periodic table.

1.1 Organic chemistry in day to day life

Organic compounds are associated with nearly every aspect of our existence. For example:

Food components: Carbohydrates, fats, proteins
Plastic materials: PVC, polythene, polystyrene, polyesters, nylon
Medicines: Paracetamol, aspirin, penicillin, amoxicillin
Fuels: Petrol, diesel, kerosene, LP gas

1.1.1 Why carbon can form a large number of organic compounds with vast structural diversity? Uniqueness of carbon

Carbon-carbon and carbon-hydrogen bonds are the predominant bonds found in organic compounds. Between two C atoms strong single bonds, double bonds and triple bonds can be formed. The small electronegativity difference between C and H also leads to the formation of C–H covalent bonds. The presence of 4 electrons in its valence shell enables it to form 4 covalent bonds which include carbon-carbon double bonds and triple bonds. Due to these reasons, carbon is capable of forming linear and branched chains and rings leading to compounds with diverse carbon skeletons. As carbon can also form bonds with O, N, S, P and halogens, this leads to the formation of an enormous variety of organic compounds having a wide range of molecular weights. When compared to Si which is also in the fourth group of the periodic table to which C belongs, the C–C and C–H bonds possess higher bond energies than Si–Si and Si–H bonds. Some bond energies relevant to the discussion above are shown in **Table 1.1.**

Table 1.1 Bond energies of some bonds with C and Si

Bond	Bond energy/ kJ mol^{-1}
C–C	346
C=C	610
C≡C	835
C–H	413
Si–Si	226
Si–H	318

1.2 Diversity of organic compounds in terms of functional groups

Some organic compounds contain only C and H as the constituent elements. They are known as hydrocarbons. On the basis of the structure, hydrocarbons are divided into two main groups called aliphatic and aromatic. Hydrocarbons consisting of only open carbon chains are called as acyclic aliphatic hydrocarbons while those with cyclic carbon chains are called alicyclic hydrocarbons. The aliphatic hydrocarbons are classified as alkanes, alkenes, and alkynes. The cyclic organic compounds which are stabilized by forming a cyclic delocalized cloud of π electrons are called aromatic compounds. Benzene which is indicated by the molecular formula C_6H_6 is the simplest of aromatic hydrocarbon compounds. The classification of hydrocarbons is shown in the **Figure 1.1** with common examples of each type.

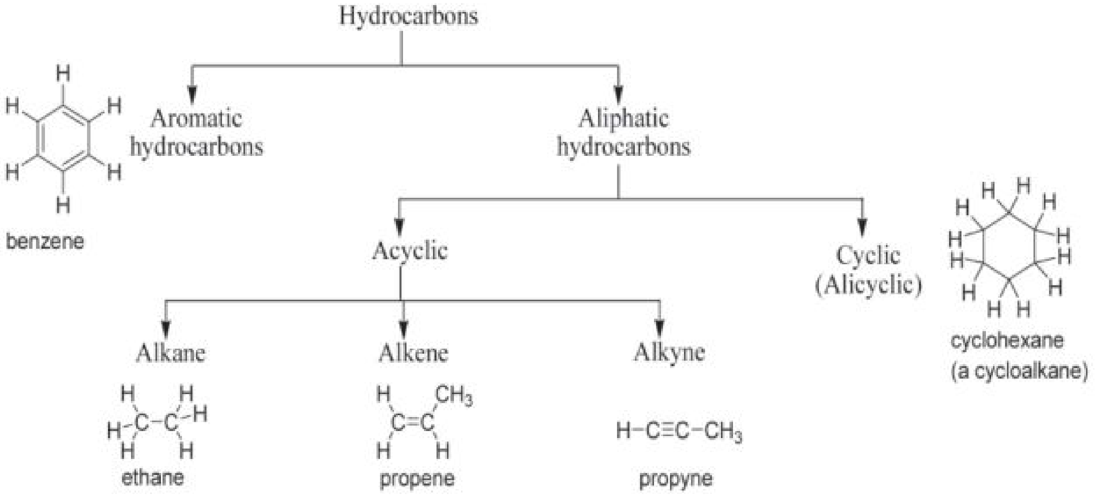
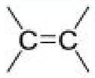
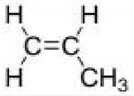
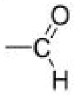
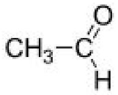
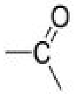
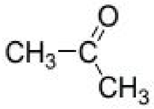
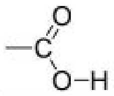
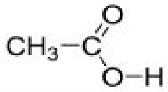
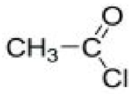
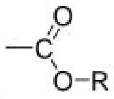
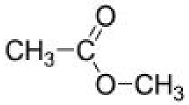
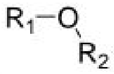
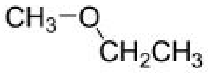
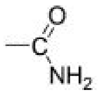
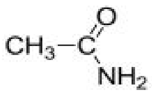
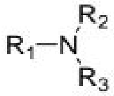
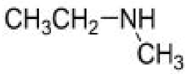


Figure 1.1 Classification of hydrocarbons

Note: *Cycloalkanes, cycloalkenes and cycloalkynes are not included in the current G.C.E. (A/L) syllabus.*

Compounds are classified according to the functional groups present in their molecules. A functional group is a group of atoms in a molecule where most of its reactions take place. Apart from the carbon-carbon double bond and carbon-carbon triple bond, a functional group contains one or more heteroatoms such as nitrogen and oxygen. Common functional groups and the names of the corresponding homologous series are given in **Table 1.2.**

Table 1.2 Functional groups in organic compounds

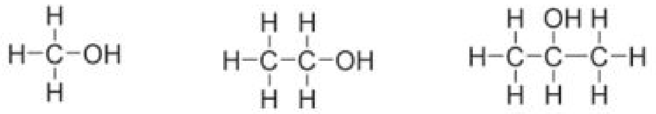
Functional group	Name of the homologous series		Example with name	
	Alkene			propene
$-C\equiv C-$	Alkyne		$H-C\equiv C-H$	ethyne
$-OH$	Alcohol		CH_3CH_2-OH	ethanol
	Aldehyde			ethanal
	Ketone			propanone
	Carboxylic acid			ethanoic acid
	Acid halide	X = Cl; acid chloride X = Br; acid bromide		ethanoyl chloride
	Ester			methyl ethanoate
	Ether			ethylmethyl ether
	Amide			ethanamide
	Amine		$CH_3CH_2-NH_2$ 	ethylamine ethylmethylamine
$-C\equiv N$	Nitrile		$CH_3CH_2-C\equiv N$	propanenitrile
$-X$	Alkyl halide	X = Cl; alkyl chloride X = Br; alkyl bromide X = I; alkyl iodide	CH_3CH_2-Cl CH_3CH_2-Br	chloroethane bromoethane

***Note:** Alkenes, alkynes, ethers and alkyl halides are not considered as functional groups in the IUPAC nomenclature system.*

1.2.1 Classes of compounds with functional groups containing heteroatoms

1.2.1.1 Alcohol

Alcohols are compounds containing a hydroxyl group (–OH) attached to an alkyl group. Some examples are given in **Figure 1.2.**



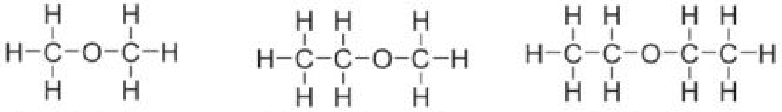
methyl alcohol ethyl alcohol *iso*-propyl alcohol

Figure 1.2 Some examples for alcohols

Note: *An alkyl group is formally derived from an alkane by the removal of a hydrogen atom.*

1.2.1.2 Ethers

Ethers are compounds containing an oxygen atom attached to two alkyl groups. Some examples are given in **Figure 1.3.**

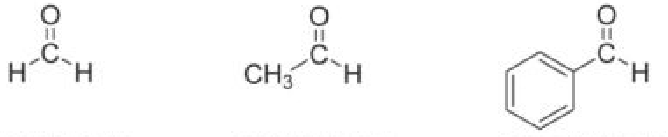


dimethyl ether ethyl methyl ether diethyl ether

Figure 1.3 Some examples for ethers

1.2.1.3 Aldehyde

Aldehydes are compounds containing a carbonyl (C=O) group attached to an H atom. Some examples are given in **Figure 1.4.**

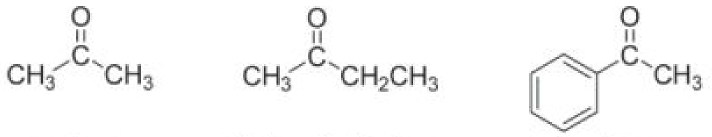


formaldehyde acetaldehyde benzaldehyde

Figure 1.4 Some examples for aldehydes

1.2.1.4 Ketones

Ketones are compounds containing a carbonyl (C=O) group attached to two carbon atoms each of which may belong to an alkyl or aryl group. Some examples are given in **Figure 1.5.**



acetone ethyl methyl ketone acetophenone

Figure 1.5 Some examples for ketones

1.2.1.5 Alkyl halides

Alkyl halides are compounds containing a halogen atom bonded to an alkyl group. Some examples are given in **Figure 1.6.**

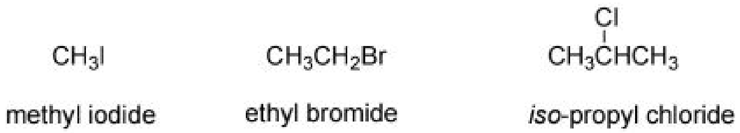


Figure 1.6 Some examples for alkyl halides

Note: *Compounds containing a halogen atom joined to an aromatic ring are called aryl halides.*

1.2.1.6 Carboxylic acids

Carboxylic acids are compounds containing the carboxylic acid (COOH) group. Some examples are given in **Figure 1.7.**

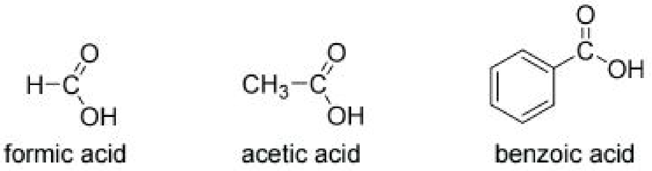


Figure 1.7 Some examples for carboxylic acids

1.2.1.7 Acid halides, esters and amides (derivatives of carboxylic acids)

Acid halides are compounds containing the COX group where X is a halogen atom. Esters are compounds containing the COOR group and amides are compounds containing the $CONH_2$ group. Some examples are given in **Figure 1.8.**

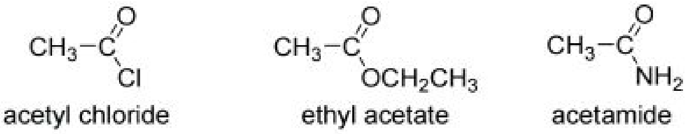


Figure 1.8 Some examples for derivatives of carboxylic acids

Note: *Acid halides, esters and amides are derived by replacing the OH group in the COOH group by halogen, OR and NH_2 groups respectively.*

1.2.1.8 Amines

Amines are compounds derived formally from ammonia by replacing its H atoms either by alkyl groups or aryl groups. Some examples are given in **Figure 1.9.**

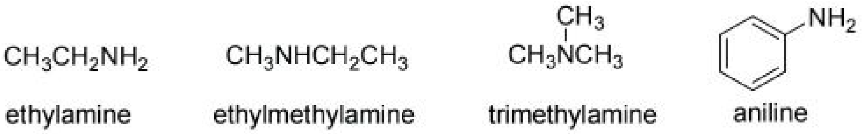


Figure 1.9 Some examples for amines

1.3 IUPAC nomenclature of organic compounds

The set of rules for systematic nomenclature of organic compounds which is now in practice evolved through several international conferences and are known as International Union of Pure and Applied Chemistry rules (IUPAC rules). Therefore, this system of nomenclature is called the IUPAC nomenclature system. In addition to the IUPAC nomenclature many common organic compounds are known by trivial (non-systematic) names. Some examples are given at the end of this section.

1.3.1 IUPAC nomenclature

The IUPAC nomenclature system is governed by a large number of rules. In our discussion we will limit ourselves to understand the most important ones which can be used to name more common types of organic compounds. The most important feature of the IUPAC system would be that it will allow us to give one name to a given organic compound and to write only one structure for a given IUPAC name.

In this system, all the compounds with heteroatoms such as O, N, halogen, are considered to be derived from the corresponding hydrocarbon. Therefore, as a start, let us look at how hydrocarbons are named according to the IUPAC system of nomenclature.

1.3.2 Alkane hydrocarbons

All the names of saturated hydrocarbons end with the suffix **-ane.** The stem of the hydrocarbon name denotes the number of carbon atoms present in the longest carbon chain. Learning the stems is like learning to count in Organic Chemistry. Stem names up to 6 carbon atoms are given in **Table 1.3.**

Table 1.3 Stem names of hydrocarbons having up to six carbon atoms

Carbon Number	Stem name	Name of hydrocarbon	Structure
1	meth-	methane	CH_4
2	eth-	ethane	CH_3CH_3
3	prop-	propane	$CH_3CH_2CH_3$
4	but-	butane	$CH_3CH_2CH_2CH_3$
5	pent-	pentane	$CH_3CH_2CH_2CH_2CH_3$
6	hex-	hexane	$CH_3CH_2CH_2CH_2CH_2CH_3$

Before we consider little more complex hydrocarbons, let us look at how we can name alkyl groups.

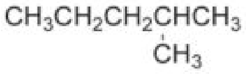
When we formally remove a H atom from an alkane an alkyl group is obtained. The name of an alkyl group ends with the suffix **-yl**. When the terminal H atom of an unbranched hydrocarbon is removed the unbranched alkyl group is formed. Some examples are given in **Table 1.4**.

Table 1.4 Some examples of alkyl groups

Hydrocarbon		Alkyl group	
$H{-}CH_3$	methane	$-CH_3$	methyl
$H{-}CH_2CH_3$	ethane	$-CH_2CH_3$	ethyl
$H{-}CH_2CH_2CH_3$	propane	$-CH_2CH_2CH_3$	propyl

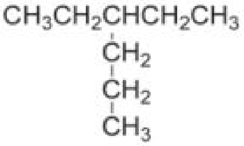
1.3.3 Nomenclature of branched chain alkanes

Branched chain alkanes can be considered the hydrocarbons which have alkyl groups attached to its longest carbon chain. Let us go through the steps involved in naming of branched chain alkanes taking the following examples.



$CH_3CH_2CH_2CH(CH_3)CH_3$

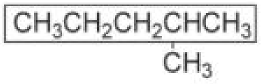
(1)



$CH_3CH_2CH(CH_2CH_2CH_3)CH_2CH_3$

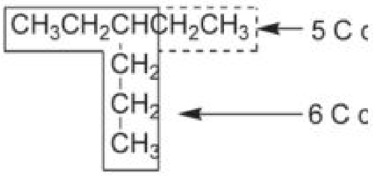
(2)

Step 1. Identify the longest continuous chain of carbon atoms and derive the hydrocarbon name.



(1)

5 Carbon atoms – pentane

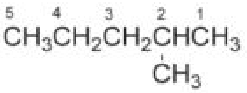


(2)

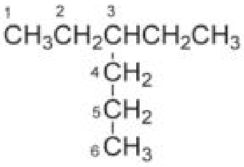
6 C atoms - hexane

Note: A methyl group is attached to one of the C atoms of compound 1 and an ethyl group is attached to one of the C atoms of compound 2. A group that replaces an H atom of the hydrocarbon chain is called a substituent group. Therefore methyl group in compound 1 and ethyl group in compound 2 are substituents.

Step 2. Number the carbon atoms of the longest continuous carbon chain such that the C atom bearing the substituent group gets the lowest possible number.



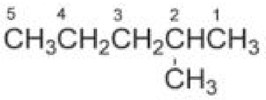
(1)



(2)

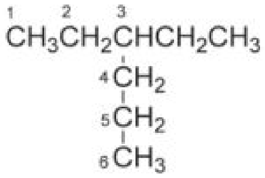
Note: *The carbon chain of compound 1is numbered from right to left. If the carbon chain of this compound is numbered from left to right, the carbon atom to which the methyl group is attached will be assigned number 4 which is a higher number than 2.*

Step 3. Use the number obtained by applying the above step (2) to designate the location of the substituent. Write the name of the compound by placing the hydrocarbon name (name of the parent hydrocarbon) at last preceded by the substituent group with the number designating its location. Numbers are separated from words by a hyphen while numbers are separated by commas.



$\overset{5}{C}H_3\overset{4}{C}H_2\overset{3}{C}H_2\underset{CH_3}{\overset{2}{C}H}\overset{1}{C}H_3$

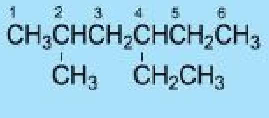
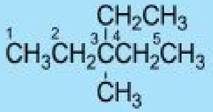
(1)
2-methylpentane



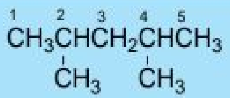
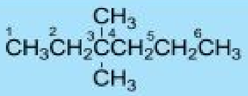
$$\begin{array}{l}\overset{1}{C}H_3\overset{2}{C}H_2\overset{3}{C}HCH_2CH_3\\ \qquad\;\; {}_4CH_2\\ \qquad\;\; {}_5CH_2\\ \qquad\;\; {}_6CH_3\end{array}$$

(2)
3-ethylhexane

When two or more substituents are present they should get the lowest possible numbers designating their location on the longest carbon chain. The substituent groups should be placed alphabetically in the IUPAC name. Let us take two more examples.

	 $\overset{1}{C}H_3\underset{CH_3}{\overset{2}{C}H}\overset{3}{C}H_2\underset{CH_2CH_3}{\overset{4}{C}H}\overset{5}{C}H_2\overset{6}{C}H_3$	 $\overset{1}{C}H_3\overset{2}{C}H_2\underset{CH_3}{\overset{CH_2CH_3}{\overset{3\,4}{C}}}\overset{5}{C}H_2CH_3$
Longest hydrocarbon chain	Six - hexane	Five - pentane
Substituents and their location	2-methyl, 4-ethyl	3-methyl, 3-ethyl
IUPAC name	4-ethyl-2-methylhexane	3-ethyl-3-methylpentane

When two or more substituents are identical, they are indicated by the prefixes, di- (2), tri- (3), tetra- (4) etc. Every substituent should be given the number that shows its location on the longest carbon chain.

	 $\overset{1}{C}H_3\underset{CH_3}{\overset{2}{C}H}\overset{3}{C}H_2\underset{CH_3}{\overset{4}{C}H}\overset{5}{C}H_3$	 $\overset{1}{C}H_3\overset{2}{C}H_2\underset{CH_3}{\overset{CH_3}{\overset{3\,4}{C}}}CH_2\overset{5}{C}H_2\overset{6}{C}H_3$
Longest hydrocarbon chain	Five - pentane	Six - hexane
Substituents and their location	2-methyl, 4-methyl	3-methyl, 3-methyl
IUPAC name	2,4-dimethylpentane	3,3-dimethylhexane

1.3.4 Nomenclature of alkene and alkyne hydrocarbons

Alkenes contain carbon-carbon double bonds. According to IUPAC nomenclature, the suffix -ane is replaced by suffix -ene in alkenes with the number designating the location of the double bond in the parent hydrocarbon. Let us go through the steps involved in naming alkenes taking some examples.

$CH_3CH_2CH=CH_2$
(3)

$CH_3CH_2CH=CHCH_3$
(4)

Step 1. Identify the longest continuous carbon chain including the carbon-carbon double bond. Number the carbon chain such that the double bond carbons get the lowest possible numbers.

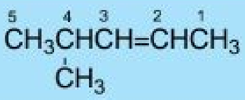
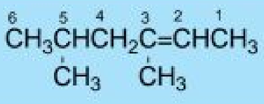
$\overset{4}{C}H_3\overset{3}{C}H_2\overset{2}{C}H=\overset{1}{C}H_2$
(3)

$\overset{5}{C}H_3\overset{4}{C}H_2\overset{3}{C}H=\overset{2}{C}H\overset{1}{C}H_3$
(4)

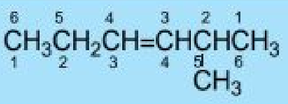
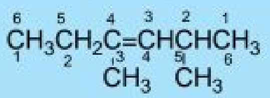
Step 2. Build the IUPAC name by placing the name representing the carbon number and suffix -ene with the lowest number designated to the location of the double bond.

	$\overset{4}{C}H_3\overset{3}{C}H_2\overset{2}{C}H=\overset{1}{C}H_2$ (3)	$\overset{5}{C}H_3\overset{4}{C}H_2\overset{3}{C}H=\overset{2}{C}H\overset{1}{C}H_3$ (4)
Longest carbon chain	Four - but	Five – pent
Double bond location	1,2	2,3
IUPAC name	but-1-ene (1-butene)	pent-2-ene (2-pentene)

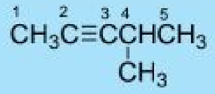
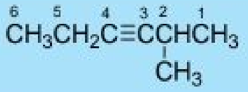
Step 3. When substituents are present, they are placed in as prefixes along with the number designated to indicate their location in the longest carbon chain containing the double bond.

	 $\overset{5}{C}H_3\underset{CH_3}{\overset{4}{C}}H\overset{3}{C}H=\overset{2}{C}H\overset{1}{C}H_3$	 $\overset{6}{C}H_3\underset{CH_3}{\overset{5}{C}}H\overset{4}{C}H_2\underset{CH_3}{\overset{3}{C}}=\overset{2}{C}H\overset{1}{C}H_3$
Longest carbon chain	Five - pent	Six - hex
Double bond location	2,3	2,3
Parent hydrocarbon name	pent-2-ene (2-pentene)	hex-2-ene (2-hexene)
Substituents with location	4-methyl	3-methyl, 5-methyl
IUPAC name	4-methylpent-2-ene (4-methyl-2-pentene)	3,5-dimethylhex-2-ene (3,5-dimethyl-2-hexene)

If the double bond gets the same set of numbers when the chain is numbered from either sides of the carbon chain, then the numbering should be done such that substituents get the lowest possible numbers.

	 $CH_3CH_2CH{=}CH\underset{\substack{\vert \\ CH_3}}{C}HCH_3$	 $CH_3CH_2\underset{\substack{\vert \\ CH_3}}{C}{=}CH\underset{\substack{\vert \\ CH_3}}{C}HCH_3$
Longest carbon chain	Six - hex	Six - hex
Double bond location	3, 4	3, 4
Parent hydrocarbon name	hex-3-ene (3-hexene)	hex-3-ene (3-hexene)
Substituents with location	2-methyl	2-methyl, 4-methyl
IUPAC name	2-methylhex-3-ene (2-methyl-3-hexene)	2,4-dimethylhex-3-ene (2,4-dimethyl-3-hexene)

Alkynes contain carbon-carbon triple bonds. They are named by replacing suffix -**ane** of alkane by suffix -**yne.** The rest follows similar to nomenclature of alkenes.

	 $CH_3C{\equiv}C\underset{\substack{\vert \\ CH_3}}{C}HCH_3$	 $CH_3CH_2C{\equiv}C\underset{\substack{\vert \\ CH_3}}{C}HCH_3$
Longest carbon chain	Five - pent	Six - hex
Triple bond location	2, 3	3, 4
Parent hydrocarbon name	pent-2-yne (2-pentyne)	hex-3-yne (3-hexyne)
Substituents with location	4-methyl	2-methyl
IUPAC name	4-methylpent-2-yne (4-methyl-2-pentyne)	2-methylhex-3-yne (2-methyl-3-hexyne)

Let us now summarize the basic principles of naming hydrocarbons according to the IUPAC system. **This will be the foundation for the naming of compounds containing functional groups.**

(i) All the compounds are considered to be derived from the hydrocarbon containing the longest carbon chain.

(ii) When a double bond or a triple bond is present, the longest carbon chain should be chosen to include the double bond or the triple bond.

(iii) A suitable suffix (-ane, -ene or -yne) is added to the stem name which denotes the number of carbon atoms (parent hydrocarbon).

(iv) When double bonds or triple bonds are absent, the carbon atoms carrying substituents are given the lowest possible numbers.

(v) When a double bond or a triple bond is present it is given the lowest possible number.

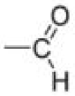
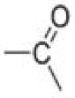
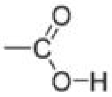
(vi) Substituent names are placed as prefixes to the parent hydrocarbon name in the alphabetical order.

1.3.5 IUPAC nomenclature of compounds other than hydrocarbons

In this section nomenclature of compounds containing other functional groups **(Table 1.2)** will be discussed. This also follows the principles we have already discussed. In addition we now need a class name (suffix) to designate the functional group present in the molecule.

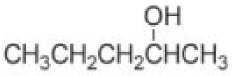
Let us take class names (suffixes) **(Table 1.5)** of some functional groups and study how these principles should be applied in naming compounds with one functional group.

Table 1.5 Class names of some functional groups

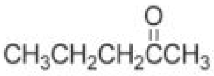
Functional group	**Name of the homologous series**	**Class name (Suffix)**
—OH	Alcohol	-ol
	Aldehyde	-al
	Ketone	-one
	Carboxylic acid	-oic acid

Let us now go through the steps involved in naming the following compounds.

$CH_3CH_2CH_2CH_2OH$

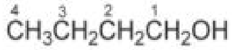


$CH_3CH_2CH_2\overset{OH}{\overset{|}{C}}HCH_3$

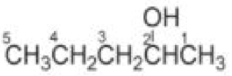


$CH_3CH_2CH_2\overset{O}{\overset{\|}{C}}CH_3$

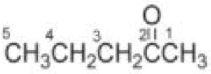
1. Identify the longest continuous carbon chain containing the functional group and number the carbon atoms of the carbon chain such that the C atom bearing the functional group gets the lowest possible number.



$\overset{4}{C}H_3\overset{3}{C}H_2\overset{2}{C}H_2\overset{1}{C}H_2OH$

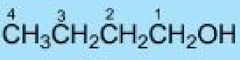
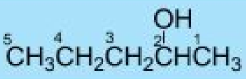
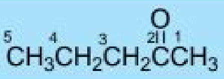


$\overset{5}{C}H_3\overset{4}{C}H_2\overset{3}{C}H_2\overset{OH}{\overset{2}{C}}H\overset{1}{C}H_3$



$\overset{5}{C}H_3\overset{4}{C}H_2\overset{3}{C}H_2\overset{O}{\overset{2}{C}}\overset{1}{C}H_3$

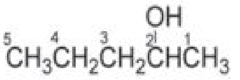
2. Derive the parent hydrocarbon name which shows the number of C atoms and whether it is saturated or contains a double bond or a triple bond.

 $\overset{4}{C}H_3\overset{3}{C}H_2\overset{2}{C}H_2\overset{1}{C}H_2OH$		 $\overset{5}{C}H_3\overset{4}{C}H_2\overset{3}{C}H_2\overset{OH}{\overset{2}{C}}H\overset{1}{C}H_3$		 $\overset{5}{C}H_3\overset{4}{C}H_2\overset{3}{C}H_2\overset{O}{\overset{2}{C}}\overset{1}{C}H_3$	
4 C atoms:	but	5 C atoms:	pent	5 C atoms:	pent
Saturated hydrocarbon chain:	ane	Saturated hydrocarbon chain:	ane	Saturated hydrocarbon chain:	ane
but + ane; butane		pent + ane; pentane		pent + ane; pentane	

3. Write the name of the compound by placing the hydrocarbon name deleting the last letter 'e' (name of the parent hydrocarbon) followed by the suffix identifying the functional group with the number designating its location.

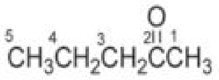
$\overset{4}{C}H_3\overset{3}{C}H_2\overset{2}{C}H_2\overset{1}{C}H_2OH$

butane + 1-ol
butan-1-ol (1-butanol)



$\overset{5}{C}H_3\overset{4}{C}H_2\overset{3}{C}H_2\overset{\overset{OH}{|}}{\overset{2}{C}}H\overset{1}{C}H_3$

pentane + 2-ol
pentan-2-ol (2-pentanol)



$\overset{5}{C}H_3\overset{4}{C}H_2\overset{3}{C}H_2\overset{\overset{O}{\|}}{\overset{2}{C}}\overset{1}{C}H_3$

pentane + 2-one
pentan-2-one (2-pentanone)

The IUPAC names derived above give the following information:

(i) The number of C atoms in the longest continuous carbon chain (pent, but etc.).

(ii) The saturated nature of the carbon chain (-an-)

(iii) The functional group present in the molecule and its position (1-ol, 2-ol or 2-one).

Note:*The hydroxyl group (OH) of alcohols can be positioned on any carbon atom including the terminal carbon atom of the carbon chain while the carbonyl group (C=O) of ketones cannot be positioned at the terminal carbon atom of the carbon chain. Thus in naming alcohols and ketones the number designating the location of the functional group has to be stated.*

The carbonyl group (C=O) of the aldehydes and the carboxylic acids are always positioned at the terminal carbon atom of the carbon chain. Therefore it is not necessary to state the number designating their location.

Let us take the following two examples.

$CH_3CH_2CH_2COOH$ $CH_3CH_2CH_2CH_2CHO$

1. Identify the longest continuous carbon chain containing the functional group and number the carbon atoms of the carbon chain such that the C atom of the functional group gets number 1.

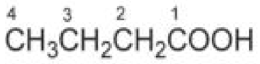
$\overset{4}{C}H_3\overset{3}{C}H_2\overset{2}{C}H_2\overset{1}{C}OOH$ $\overset{5}{C}H_3\overset{4}{C}H_2\overset{3}{C}H_2\overset{2}{C}H_2\overset{1}{C}HO$

2. Derive the parent hydrocarbon name which shows the number of C atoms and whether it is saturated or contains a double bond or a triple bond.

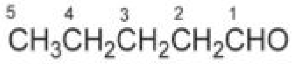
$\overset{4}{C}H_3\overset{3}{C}H_2\overset{2}{C}H_2\overset{1}{C}OOH$
4 C atoms and saturated
hydrocarbon (but + ane)

$\overset{5}{C}H_3\overset{4}{C}H_2\overset{3}{C}H_2\overset{2}{C}H_2\overset{1}{C}HO$
5 C atoms and saturated
hydrocarbon (pent + ane)

3. Write the name of the compound by placing the hydrocarbon name deleting the last letter ‘e’ (name of the parent hydrocarbon) followed by the suffix identifying the functional group. Because aldehyde functional group and carboxylic acid functional group always get number 1, the number is not stated in the name.

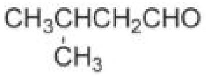

$\overset{4}{C}H_3\overset{3}{C}H_2\overset{2}{C}H_2\overset{1}{C}OOH$

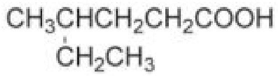
butane + oic acid
butanoic acid


$\overset{5}{C}H_3\overset{4}{C}H_2\overset{3}{C}H_2\overset{2}{C}H_2\overset{1}{C}HO$

pentane + al
pentanal

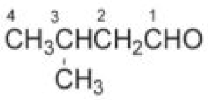
Let us now take few examples containing alkyl substituents attached to the longest continuous carbon chain. Recall that aldehyde and carboxylic acid functional groups are always positioned at the terminal of the carbon chain. Hence the C of these two functional groups is given number 1 when numbering.

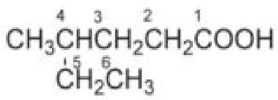

$CH_3\underset{CH_3}{CH}CH_2CHO$


$CH_3\underset{CH_2CH_3}{CH}CH_2CH_2COOH$

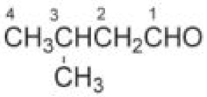
Let us go through the steps involved in naming the above examples.

1. Identify the longest continuous carbon chain containing the functional group and number the carbon atoms of the carbon chain such that the C atom of the functional group gets number 1.

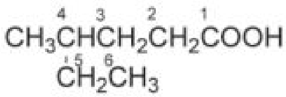

$\overset{4}{C}H_3\underset{CH_3}{\overset{3}{C}H}\overset{2}{C}H_2\overset{1}{C}HO$


$CH_3\underset{\overset{5}{C}H_2\overset{6}{C}H_3}{\overset{4}{C}H}\overset{3}{C}H_2\overset{2}{C}H_2\overset{1}{C}OOH$

2. Derive the parent hydrocarbon name which shows the number of C atoms and whether it is saturated or contains a double bond or a triple bond.

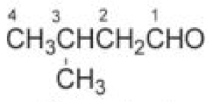

$\overset{4}{C}H_3\underset{CH_3}{\overset{3}{C}H}\overset{2}{C}H_2\overset{1}{C}HO$

4 C atoms and saturated
hydrocarbon (but + ane)

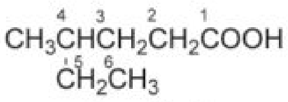

$CH_3\underset{\overset{5}{C}H_2\overset{6}{C}H_3}{\overset{4}{C}H}\overset{3}{C}H_2\overset{2}{C}H_2\overset{1}{C}OOH$

6 C atoms and saturated
hydrocarbon (hex+ ane)

3. Identify the substituent groups with the location.

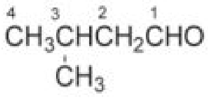

$\overset{4}{C}H_3\underset{CH_3}{\overset{3}{C}H}\overset{2}{C}H_2\overset{1}{C}HO$

3-methyl

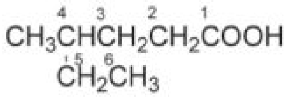

$CH_3\underset{\overset{5}{C}H_2\overset{6}{C}H_3}{\overset{4}{C}H}\overset{3}{C}H_2\overset{2}{C}H_2\overset{1}{C}OOH$

4-methyl

4. Build the IUPAC name of the compound by placing the hydrocarbon name deleting the last letter 'e' (name of the parent hydrocarbon) followed by the suffix identifying the functional group. Place the substituent names with their locations as prefixes. When there are several substituents they should be placed in the alphabetical order.

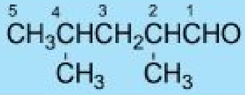
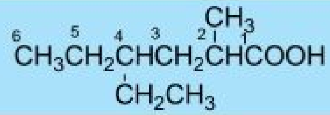

$\overset{4}{C}H_3\underset{CH_3}{\overset{3}{C}H}\overset{2}{C}H_2\overset{1}{C}HO$

3-methyl+butane+al
3-methylbutanal


$CH_3\underset{\overset{5}{C}H_2\overset{6}{C}H_3}{\overset{4}{C}H}\overset{3}{C}H_2\overset{2}{C}H_2\overset{1}{C}OOH$

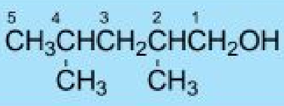
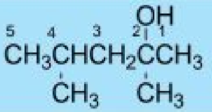
4-methyl+hexane+oic acid
4-methylhexanoic acid

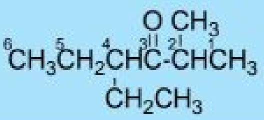
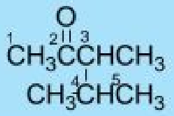
Let us take two more examples.

	 $CH_3\underset{CH_3}{CH}CH_2\underset{CH_3}{CH}CHO$	 $CH_3CH_2\underset{CH_2CH_3}{CH}CH_2\overset{CH_3}{CH}COOH$
Longest carbon chain	5C – pent	6C - hex
Parent hydrocarbon name	pentane	hexane
Functional group (with location)	1-al	1-oic acid
Substituents with locations	2-methyl, 4-methyl	2-methyl, 4-ethyl
IUPAC name	2,4-dimethylpentanal	4-ethyl-2-methylhexanoic acid

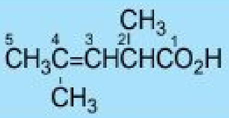
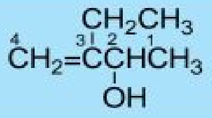
Carbon chains of compounds containing functional groups that can be placed on any carbon atom (such as alcohols and ketones) should be numbered such that the functional group gets the lowest possible number. Rest of the steps discussed will then be followed to build the IUPAC name.

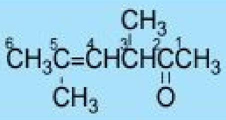
Let us take few examples.

	 $CH_3\underset{CH_3}{CH}CH_2\underset{CH_3}{CH}CH_2OH$	 $CH_3\underset{CH_3}{CH}CH_2\overset{OH}{\underset{CH_3}{C}}CH_3$
Longest carbon chain	5C atoms - pent	5C atoms - pent
Parent hydrocarbon name	pentane	pentane
Functional group (with location)	OH at C-1 (1-ol)	OH at C-2 (2-ol)
Substituents with locations	2-methyl, 4-methyl	2-methyl, 4-methyl
IUPAC name	2,4-dimethylpentan-1-ol 2,4-dimethy- lpentanol	2,4-dimethylpentan-2-ol 2,4-dimethyl-2-pentanol

	 $CH_3CH_2\underset{CH_2CH_3}{CH}\overset{O}{\overset{\|}{C}}-\overset{CH_3}{CH}CH_3$	 $CH_3\overset{O}{\overset{\|}{C}}\underset{CH_3CHCH_3}{CH}CH_3$
Longest carbon chain	6C atoms - hex	5C atoms - pent
Parent hydrocarbon name	hexane	pentane
Functional group (with location)	C=O at C-3 (3-one)	C=O at C-2 (2-one)
Substituents with locations	2-methyl, 4-ethyl	3-methyl, 4-methyl
IUPAC name	4-ethyl-2-methylhexan-3-one 4-ethyl-2-methyl-3-hexanone	3,4-dimethylpentan-2-one 3,4-dimethyl-2-pentanone

When the compound contains a double bond or a triple bond (a multiple bond), the longest chain must contain both the functional group and the multiple bond. Accordingly the parent hydrocarbon will be either an alkene or an alkyne. Rest of the steps discussed will then be followed to build the IUPAC name. Let us take a look at few examples.

	 $\overset{5}{C}H_3\underset{CH_3}{\overset{4}{C}}=\overset{3}{C}H\overset{CH_3}{\overset{2}{C}}H\overset{1}{C}O_2H$	 $\overset{4}{C}H_2=\overset{CH_2CH_3}{\overset{3}{C}}\underset{OH}{\overset{2}{C}}H\overset{1}{C}H_3$
Longest carbon chain	5C atoms - pent	4C atoms - but
Functional group with location	oic acid	2-ol
Double/triple bond with location	3-ene	3-ene
Parent hydrocarbon name	pent-3-ene	but-3-ene
Substituents with locations	2-methyl, 4-methyl	3-ethyl
IUPAC name	2,4-dimethylpent-3-enoic acid 2,4-dimethyl-3-pentenoic acid	3-ethylbut-3-en-2-ol 3-ethyl-3-buten-2-ol

	 $\overset{6}{C}H_3\underset{CH_3}{\overset{5}{C}}=\overset{4}{C}H\overset{CH_3}{\overset{3}{C}}H\underset{O}{\underset{\|}{\overset{2}{C}}}\overset{1}{C}H_3$	 $\overset{6}{C}H_3\overset{5}{C}\equiv\overset{4}{C}\overset{CH_3}{\overset{3}{C}}H\overset{2}{C}H_2\overset{1}{C}HO$
Longest carbon chain	6C atoms - hex	6C atoms - hex
Functional group with location	2-one	al
Double/triple bond with location	4-ene	4-yne
Parent hydrocarbon name	hex-4-ene	hex-4-yne
Substituents with locations	3-methyl, 5-methyl	3-methyl
IUPAC name	3,5-dimethylhex-4-en-2-one	3-methylhex-4-ynal
	3,5-dimethyl-4-hexen-2-one	3-methyl-4-hexynal

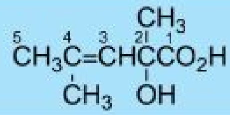
1.3.6 IUPAC nomenclature of compounds containing more than one functional group

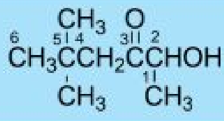
There are many organic compounds containing several functional groups. Recall that in the foregoing discussion you learnt that compounds are named according to their functional group. In the IUPAC nomenclature system, functional groups are arranged in a priority order. When there are two functional groups in a molecule, the compound is named according to the functional group that gets the highest priority. The functional group with the highest priority is called the principal functional group. The remaining functional group is considered as a substituent. When a functional group is considered as substituent, it is given a different name to be used as a prefix. The carbon chain is numbered so that the principal functional group gets the lowest possible number. Class names and substituent names of some functional groups are given in **Table 1.6** in the order of their priority.

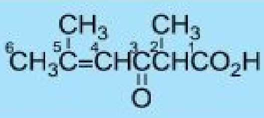
Table 1.6 Class names and substituent names of some functional groups in their priority order

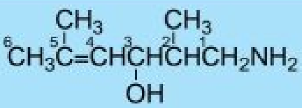
Functional group	Name of the homologous series	Substituent name (prefix)	Class name (suffix)
-COOH	Carboxylic acid	-	oic acid
-COOR	Ester	-	oate
-COCl	Acid chloride	-	oyl chloride
$-CONH_2$	Amide	-	amide
-CN	Nitrile	cyano	nitrile
-CHO	Aldehyde	formyl	al
-CO-	Ketone	oxo	one
-OH	Alcohol	hydroxy-	ol
$-NH_2$	Amine	amino	amine
-F		fluoro-	-
-Cl		chloro-	-
-Br		bromo-	-
-I		iodo-	-
$-NO_2$		nitro	-

***Note:** alkene (C=C) as "ene" and alkyne (C≡C) as "yne" are used as suffixes.*

	 $\overset{5}{C}H_3\overset{4}{C}(CH_3)=\overset{3}{C}H\overset{2}{C}(CH_3)(OH)\overset{1}{C}O_2H$
Longest carbon chain	5C atoms - pent
Functional group with highest priority and its location	oic acid
Double/triple bond with location	3-ene
Parent hydrocarbon name	pent-3-ene
Substituents with locations	2-hydroxy, 2-methyl, 4-methyl
IUPAC name	2-hydroxy-2,4-dimethylpent-3-enoic acid 2-hydroxy-2,4-dimethyl-3-pentenoic acid

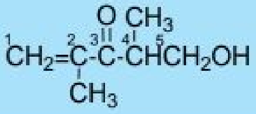
	 $CH_3\underset{CH_3}{\overset{CH_3}{C}}CH_2\overset{O}{C}\underset{CH_3}{C}HOH$
Longest carbon chain	6C atoms - hex
Functional group with highest priority and its location	3-one
Double/triple bond with location	none
Parent hydrocarbon name	hexane
Substituents with locations	2-hydroxy, 5,5-dimethyl
IUPAC name	2-hydroxy-5,5-dimethylhexan-3-one 2-hydroxy-5,5-dimethyl-3-hexanone

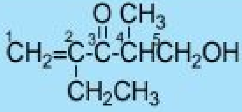
	 $CH_3\overset{CH_3}{C}=CH\underset{O}{C}\overset{CH_3}{C}HCO_2H$
Longest carbon chain	6C atoms - hex
Functional group with highest priority and its location	oic acid
Double/triple bond with location	4-ene
Parent hydrocarbon name	hex-4-ene (4-hexene)
Substituents with locations	3-oxo, 2-methyl, 5-methyl
IUPAC name	2,5-dimethyl-3-oxohex-4-enoic acid 2,5-dimethyl-3-oxo-4-hexenoic acid

	 $CH_3\overset{CH_3}{C}=CH\underset{OH}{C}H\overset{CH_3}{C}HCH_2NH_2$
Longest carbon chain	6C atoms - hex
Functional group with highest priority and its location	3-ol
Double/triple bond with location	4-ene
Parent hydrocarbon name	hex-4-ene (4-hexene)
Substituents with locations	1-amino, 2,5-dimethyl
IUPAC name	1-amino-2,5-dimethylhex-4-en-3-ol 1-amino-2,5-dimethyl-4-hexen-3-ol

	 $CH_3CH(CH_3)COCH_2CH_2OH$
Longest carbon chain	5C atoms - pent
Functional group with highest priority and its location	3-one (when numbered from either side) In such a case, the direction of numbering is chosen so as to give the lowest possible numbers to the substituent groups.
Parent hydrocarbon name	pentane
Substituents with locations	1-hydroxy, 4-methyl
IUPAC name	1-hydroxy-4-methylpentan-3-one 1-hydroxy-4-methyl-3-pentanone

	 $CH_2=CHCH(OH)CH_2CH_3$
Longest carbon chain	5C atoms - pent
Functional group with highest priority and its location	3-ol (when numbered from either side) In this case, we should give the lowest possible number to the double bond.
Double/triple bond with location	1-ene
Parent hydrocarbon name	pent-1-ene (1-pentene)
Substituents with locations	none
IUPAC name	pent-1-en-3-ol 1-penten-3-ol

	 $CH_2=C(CH_3)COCH(CH_3)CH_2OH$
Longest carbon chain	5C atoms - pent
Functional group with highest priority and its location	3-one (when numbered from either side). The lowest possible number should be given to the double bond. Recall how the substituted alkene and alkynes were named.
Double/triple bond with location	1-ene
Parent hydrocarbon name	pent-1-ene (1-pentene)
Substituents with locations	5-hydroxy, 2,4-dimethyl
IUPAC name	5-hydroxy-2,4-dimethylpent-1-en-3-one 5-hydroxy-2,4-dimethyl-1-penten-3-one

	 $\overset{1}{C}H_2=\underset{CH_2CH_3}{\overset{2}{C}}-\overset{O}{\overset{\|}{\overset{3}{C}}}-\overset{CH_3}{\overset{4}{C}H}\overset{5}{C}H_2OH$
Longest carbon chain	5C atoms - pent (not hex; the carbon chain should include the C=C).
Functional group with highest priority and its location	3-one
Double/triple bond with location	1-ene
Parent hydrocarbon name	pent-1-ene (1-pentene)
Substituents with locations	5-hydroxy, 2-ethyl, 4-methyl
IUPAC name	2-ethyl-5-hydroxy-4-methylpent-1-en-3-one 2-ethyl-5-hydroxy-4-methyl-1-penten-3-one

Let us now summarize the stepwise approach to build the IUPAC name of a compound (other than hydrocarbons).

1. Identify the longest hydrocarbon chain which includes the functional group having the highest priority (principal functional group) (Table 1.6) and any double or triple bonds.
2. Number the hydrocarbon chain:
   a. Such that the principal functional group gets the lowest possible number.
   b. If the principal functional group gets the same number when the hydrocarbon chain is numbered from different directions, then the direction giving the lowest possible number to the multiple bond is chosen.
   c. If the principal functional group gets the same number when the hydrocarbon chain is numbered from different directions and multiple bonds are absent, then the direction giving the lowest possible numbers to the substituents is chosen.
3. Derive the hydrocarbon name using the name designated for the number of C atoms and suffix for the saturation or unsaturation with its position number (ane, ene or yne).
4. Add the suffix designating the principal functional group.
5. Add prefixes designating the substituent groups along with their position numbers.
6. Then build the IUPAC name as follows:

Prefix	+	**Hydrocarbon name**	+	**Suffix**
Substituent groups with position numbers		Number of C atoms and suffix for the saturation or unsaturation with its position number		Class name of the principal functional group

Trivial Names

Prior to the development of systematic nomenclature organic compound were known by trivial (common) names. As the trivial names of common compounds are still used by chemists it is advisable to be familiar with these names. Trivial names of some common compounds and their corresponding IUPAC names are given in **Table 1.7.**

Table 1.7 Trivial names of some common compounds and their IUPAC names.

Compound	Trivial name	IUPAC name
CH_3COOH	acetic acid	ethanoic acid
CH_3CHO	acetaldehyde	ethanal
CH_3COCH_3	acetone	propanone
CH_3CN	acetonitrile	ethanenitrile
$HC{\equiv}CH$	acetylene	ethyne
$CHCl_3$	chloroform	trichloromethane
$HOCH_2CH_2OH$	ethylene glycol	ethane-1,2-diol
$HCHO$	formaldehyde	methanal
$HCOOH$	formic acid	methanoic acid

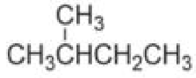
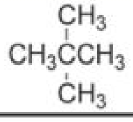
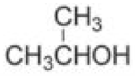
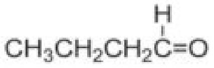
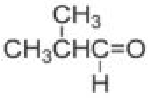
1.4 Isomerism

Isomerism is the existence of different compounds that have the **same molecular formula.** Different compounds having the same molecular formula are called isomers. Isomers can be subdivided into constitutional isomers and stereoisomers.

1.4.1 Constitutional (structural) isomerism

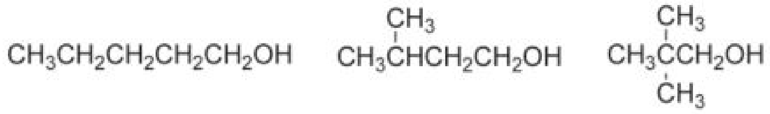
Isomers that differ from the order in which the constituent atoms are connected to each other are called **constitutional isomers.** Hence they have different structural formulae. A few examples of constitutional isomers are shown in **Table 1.8**.

Table 1.8 Some examples of constitutional isomers

Molecular formula	Constitutional isomers		
C_5H_{12}	$CH_3CH_2CH_2CH_2CH_3$	 $CH_3\overset{CH_3}{\overset{\vert}{C}}HCH_2CH_3$	 $CH_3\underset{CH_3}{\overset{CH_3}{C}}CH_3$
C_3H_8O	$CH_3CH_2CH_2OH$	 $CH_3\overset{CH_3}{\overset{\vert}{C}}HOH$	$CH_3CH_2OCH_3$
C_4H_8O	 $CH_3CH_2CH_2\overset{H}{\overset{\vert}{C}}{=}O$	 $CH_3\overset{CH_3}{\overset{\vert}{C}}H\underset{H}{C}{=}O$	 $CH_3CH_2\overset{CH_3}{\overset{\vert}{C}}{=}O$

Constitutional isomers are generally subdivided into *chain isomers, position isomers and functional group isomers*. These subdivisions are not exclusive and can overlap.

Chain isomers: Chain isomers are those which have different hydrocarbon chains for same molecular formula **(Figure 1.10).**



$CH_3CH_2CH_2CH_2CH_2OH$ $\quad CH_3\overset{CH_3}{\overset{|}{C}}HCH_2CH_2OH$ $\quad CH_3\overset{CH_3}{\overset{|}{\underset{\underset{CH_3}{|}}{C}}}CH_2OH$

Figure 1.10 Chain isomers for the molecular formula $C_5H_{12}O$

Position isomers: Position isomers are those which have the same functional group and/or substituents in different positions in the same carbon chain **(Figure 1.11)**.

$CH_3CH_2CH_2OH$ $\quad CH_3\overset{OH}{\overset{|}{C}}HCH_3$ $\quad CH_3CH_2C{\equiv}CH$ $\quad CH_3C{\equiv}CCH_3$

1-propanol 2-propanol 1-butyne 2-butyne

Position isomers for the molecular formula C_3H_8O

Position isomers for the molecular formula C_4H_6

Figure 1.11 Examples of position isomers

Functional group isomers: Functional group isomers are those which have different functional groups in compounds having the same molecular formula **(Figure 1.12).**

$CH_3CH_2CH_2OH$ $\quad CH_3CH_2OCH_3$ $\quad CH_3CH_2\overset{O}{\overset{\|}{C}}H$ $\quad CH_3\overset{O}{\overset{\|}{C}}CH_3$

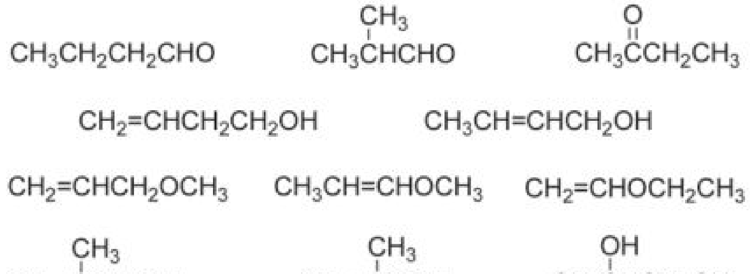
1-propanol ethylmethylether propanal propanone

Functional group isomers for the molecular formula C_3H_8O

Functional group isomers for the molecular formula C_3H_6O

Figure 1.12 Examples of functional group isomers

Chain isomerism, position isomerism and functional group isomerism can overlap. Take a look at the isomers which have been drawn for the molecular formula C_4H_8O **(Figure 1.13)**.



$CH_3CH_2CH_2CHO$ $\quad CH_3\overset{CH_3}{\overset{|}{C}}HCHO$ $\quad CH_3\overset{O}{\overset{\|}{C}}CH_2CH_3$

$CH_2{=}CHCH_2CH_2OH$ $\quad CH_3CH{=}CHCH_2OH$

$CH_2{=}CHCH_2OCH_3$ $\quad CH_3CH{=}CHOCH_3$ $\quad CH_2{=}CHOCH_2CH_3$

$CH_2{=}\overset{CH_3}{\overset{|}{C}}CH_2OH$ $\quad CH_2{=}\overset{CH_3}{\overset{|}{C}}OCH_3$ $\quad CH_3\overset{OH}{\overset{|}{C}}HCH{=}CH_2$

Figure 1.13 Constitutional isomers for the molecular formula C_4H_8O

1.4.2 Stereoisomerism

Stereoisomerism is the existence of compounds whose structures differ from each other only in the orientation of bonds in three-dimensional space. **Stereoisomers** have the same structural formulae. They have the same connectivity: their constituent atoms are connected in the same order but differ in the manner in which atoms or groups are arranged in three-dimensional space. Therefore their structures cannot be **superimposed** on each other even though they have the same molecular and structural formulae. Pair of stereoisomers whose three-dimensional structures are mirror images of each other are **enantiomers** of each other. Pairs of stereoisomers whose three-dimensional structures are not mirror images of each other are **diastereomers** of each other.

The different types of isomers described above and their classification is shown in **Figure 1.14.**

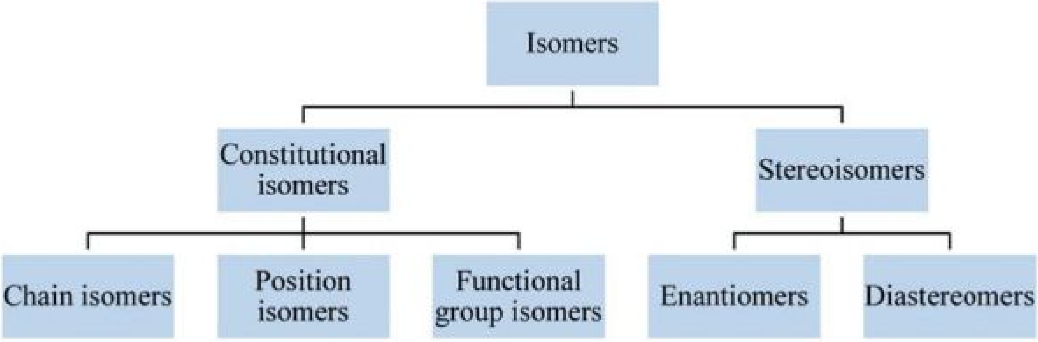
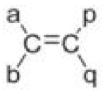


Figure 1.14 Classification of isomers

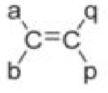
Diastereomerism

Geometric isomerism is one occasion where diastereomerism is seen. A C=C double bond consists of a σ-bond and a π-bond. Due to the π bond, the two carbon atoms cannot freely rotate about the σ-bond. Both alkene carbon atoms and the four atoms attached to them are all in one plane. For geometrical isomers to exist, the two groups attached to each carbon atom of the double bond should not be identical. In such an instance it is possible to have two compounds which differ from each other in the spatial arrangements of the groups joined to the two carbon atoms. These two compounds cannot be superimposed on each other and cannot interconvert by rotation around the carbon-carbon bond axis (due to the π-bond). Such compounds are known as geometrical isomers.

For example,

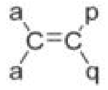


and

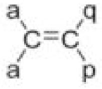


are diastereoisomers because the structures cannot be superimposed on each other.

However,



and



are the same because the structures can be superimposed on each other.

Cis and *trans* nomenclature

In alkenes the words *cis* and *trans* are used to indicate the geometrical relationship of two groups attached to different carbon atoms in the same double bond. Consider a plane passing through the C=C which is perpendicular to the plane of the molecule (See Figure 1.15). If the two groups are on the same side of this plane, then the relationship is *cis*. Observe that in **Figure 1.15** the two H-atoms are *cis* to each other and the two methyls are also *cis* to each other.

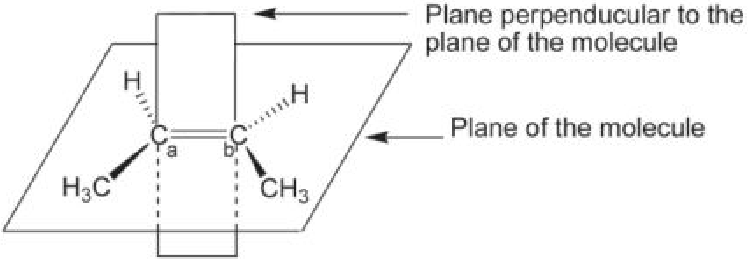


Figure 1.15 *cis*-2-butene showing the plane perpendicular to the plane of the molecule

If the two groups are on opposite sides of the plane then the relationship is *trans*. Observe that H atom on C_a is *trans* to the methyl group on C_b (see **Figure 1.16**).

Note that the geometrical isomer of *cis*-2-butene is *trans*-2-butene in which the two methyl groups are *trans* to each other (the two H atoms are also *trans* to each other).

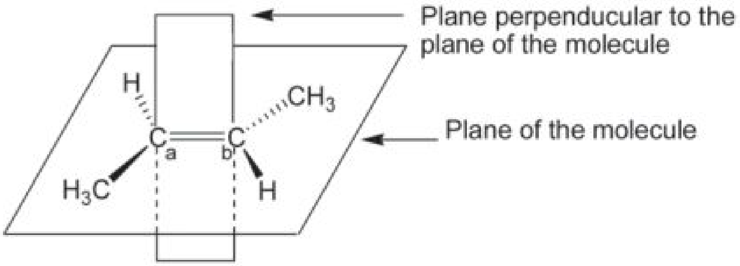


Figure 1.16 *trans*-2-butene

Enantiomerism

Isomers which are mirror images of each other are known as enantiomers (see **Figure 1.17**). A compound having a carbon atom which is joined to four different groups shows enantiomerism. Such a carbon atom is known as an asymmetric or chiral carbon atom. When plane polarized light is passed through a solution containing only one enantiomer, the plane of polarization rotates.

One enantiomer rotates the plane of polarization in one direction and the other enantiomer in the opposite direction. As the enantiomers rotate the plane of polarization, they are also known as optical isomers. Compounds which rotate the plane of plane polarized light are known as optically active compounds.

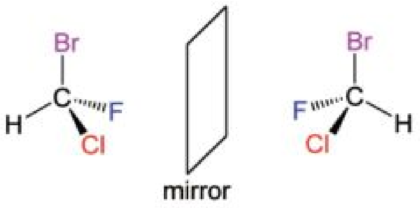


Figure 1.17 Enantiomers of bromochlorofluoromethane

Observe that the above mirror images of each other are not superimposable.

Note: *Stereoisomers which are not mirror images of each other are known as diastereomers. Therefore geometrical isomers are diastereomers.*