01 IUPAC Nomenclature and Common Names

History :

In 1675, Nicholas Lemery divided chemical substances into 3 parts.

(i) **Mineral substance :** which are obtained from minerals. eg. gold, silver, iron etc.

(ii) **Vegetable substance :** which are obtained from vegetables. eg. sugar, citric acid etc.

(iii) **Animal substance :** which are obtained from animals. eg. albumin, gilatin etc.

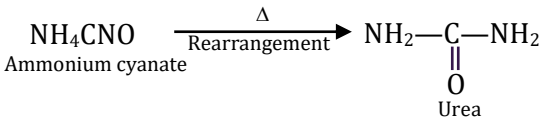
After some time when many of the chemical substance were discovered, it was found that some of them can be obtained from both vegetables and animals. So this classification was failed. So chemical substance were then divided into two parts :

(i) **Organic compounds :** which are obtained from living organism.

(ii) **Inorganic compounds :** compounds which are obtained from any other sources except living organisms.

VFT(Vital Force Theory) : By Berzelius in 1815. Upto 1815, any organic compound could not be synthesized in lab. So Berzelius suggested that there is a mysterious force in living organisms which was named as Vital Force and said that organic compounds cannot be synthesized in lab. This theory was called as VFT.

But in 1828 a German scientist Wholar synthesized an organic compound in lab. Which was 'urea'. So VFT was failed. Urea was synthesized in lab by heating of Ammonium cyanate (NH_4CNO).



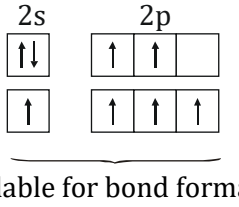
Organic Compounds : Hydrocarbons and their derivatives are called as organic compounds.

Characteristics of C-Atoms :

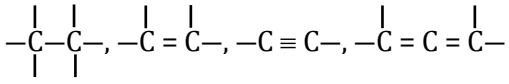
(a) Tetra valency : Atomic number of carbon atom is 6 and it have four valency electrons so C-Atom is tetravalent. It is explained by promotion rule

In ground state (here covalency of carbon is 2)

First excited state (here covalency of carbon is 4)

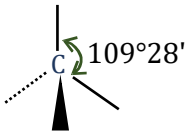


(b) Tendency to form multiple bonds : Carbon atom forms following type of bonds, such as



(c) Tetrahedral shape : The four covalent bond are directed towards the four corners of a regular tetrahedron

Bond angle 109°28' or 109.5'



(d) Catenation : Carbon atoms have the tendency to link with one another through covalent bonds to form chains and rings. This property is called catenation. This is because C—C bonds are very strong. Down the group the size increases and electronegativity decreases, and, thereby, tendency to show catenation decreases. This can be clearly seen from bond enthalpies values. The order of catenation is C > > Si > Ge ≈ Sn. Lead does not show catenation.

Due to property of catenation and pπ– pπ bond formation, carbon is able to show allotropic forms.

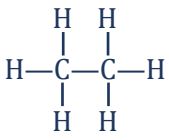
Bond	Bond enthalpy / kJ mol^{-1}
C—C	348
Si—Si	297
Ge—Ge	260
Sn—Sn	240

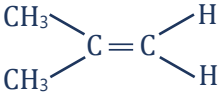
(e) Hybridisation : The orbitals of different shape but almost of equal energies blend up to give the same number of new orbitals of another shape and of identical energies.

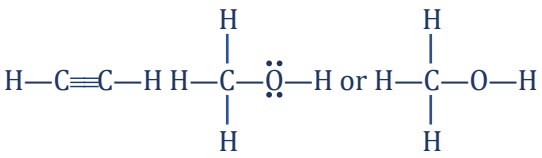
Structure	σ & π bonds	Hybridisation	Bond angle	Shape
$-\overset{\vert}{\underset{\vert}{C}}-$	4,0	sp^3	109°28'	Tetrahedral
$-\overset{\vert}{C}=$	3,1	sp^2	120°	Planar (Trigonal)
$-C\equiv$	2,2	sp	180°	Linear
$=C=$	2,2	sp	180°	Linear

Structural representations of organic compounds :

Complete, Condensed and Bond-line Structural Formulas of organic compounds are represented in several ways. The Lewis structure or dot structure, dash structure, condensed structure and bond line structural formulas are some of the specific types. The Lewis structures, however, can be simplified by representing the two-electron covalent bond by a dash (–). Such a structural formula focuses on the electrons involved in bond formation. A single dash represents a single bond, double dash is used for double bond and a triple dash represents triple bond. Lone-pairs of electrons on heteroatoms (e.g., oxygen, nitrogen, sulphur, halogens etc.) may or may not be shown. Thus, ethane (C_2H_6), ethene (C_2H_4), ethyne (C_2H_2) and methanol (CH_3OH) can be represented by the following structural formulas. Such structural representations are called complete structural formulas.


Ethane


Ethene



Ethyne Methanol

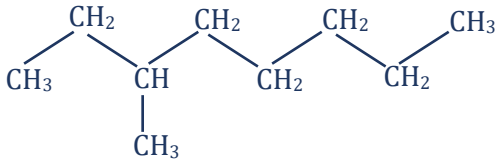
These structural formulas can be further abbreviated by omitting some or all of the dashes representing covalent bonds and by indicating the number of identical groups attached to an atom by a subscript. The resulting expression of the compound is called a condensed structural formula. Thus, ethane, ethene, ethyne and methanol can be written as:

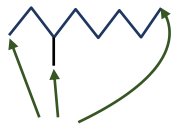
CH_3CH_3	$H_2C=CH_2$	$HC\equiv CH$	CH_3OH
Ethane	Ethene	Ethyne	Methanol

Similarly, $CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_3$ can be further condensed to $CH_3(CH_2)_6CH_3$. For further simplification, organic chemists use another way of representing the structures, in which only lines are used. In this bond-line structural representation of organic compounds, carbon and hydrogen atoms are not shown and the lines representing carbon-carbon bonds are drawn in a zig-zag fashion. The only atoms specifically written are oxygen, chlorine, nitrogen etc. The terminals denote methyl ($-CH_3$) groups (unless indicated otherwise by a functional group), while the line junctions denote carbon atoms bonded to appropriate number of hydrogens required to satisfy the valency of the carbon atoms. Some of the examples are represented as follows:

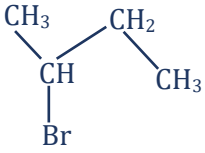
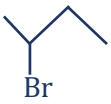
(i) 3-Methyloctane can be represented in various forms as:

(a) $CH_3CH_2CHCH_2CH_2CH_2CH_2C$ with CH_3 branch

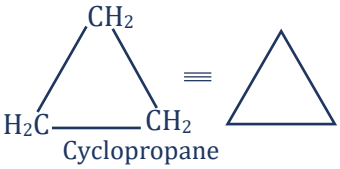
(b) 

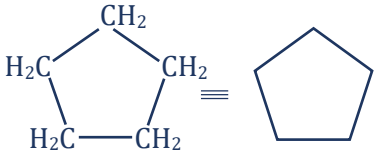
(c) 

(ii) Various ways of representing 2-bromo butane are:

(a) $CH_3CHBrCH_2CH_3$ (b)  (c) 

In cyclic compounds, the bond-line formulas may be given as follows:





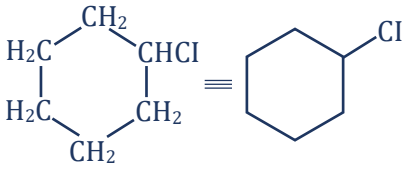
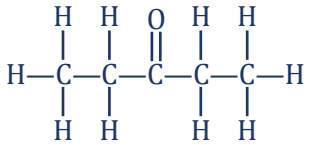


Illustration 1:

Expand each of the following condensed formulas into their complete structural formulas.

(a) $CH_3CH_2COCH_2CH_3$ (b) $CH_3CH=CH(CH_2)_3CH_3$

Solution:

(a) 

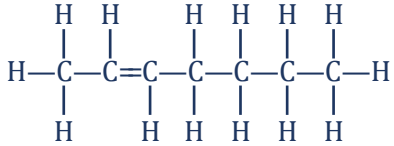
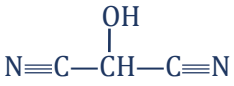
(b) 

Illustration 2 :

For each of the following compounds, write a condensed formula and also their bond-line formula.

(a) $HOCH_2CH_2CH_2CH(CH_3)CH(CH_3)CH_3$

(b) 

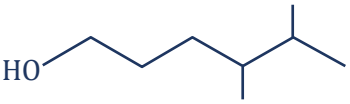
Solution:

Condensed formula:

(a) $HO(CH_2)_3CH(CH_3)CH(CH_3)_2$

(b) $HOCH(CN)_2$

Bond-line formula:

(a) 

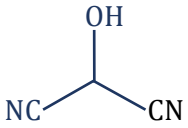
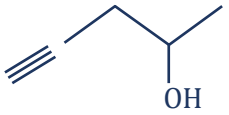
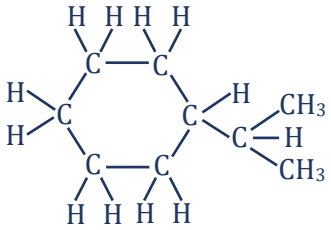
(b) 

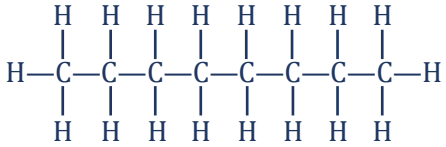
Illustration 3:

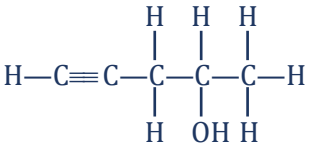
Expand each of the following bond-line formulas to show all the atoms including carbon and hydrogen

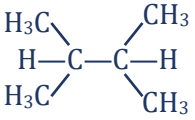
(a)  (b)  (c)  (d) 

Solution:

(a) 

(b) 

(c) 

(d) 

σ - (sigma) bonds : The molecular orbital formed by the overlapping of two-s atomic orbitals or one s and one p atomic orbitals or co-axial overlapping of p-orbitals is called a σ bond.

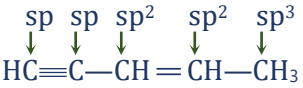
Note :

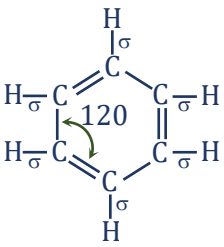
(i) Overlapping of hybrid orbitals also give σ bonds. σ bonds are stronger, as they are resulted from the effective axial overlapping.

(ii) More the directional character (p) in covalent bond more is the strength of the bond.

$sp^3 - sp^3 > sp^3 - sp^2 > sp^2 - sp^2 > sp - sp$

π(Pi) bonds : π bond is formed by the lateral overlapping of two p-atomic orbitals. It is weaker than σ bond, as there is only partial overlapping.

Ex. 

Ex.  Flat hexagonal structure due to sp^2 hybridised C-atom in benzene

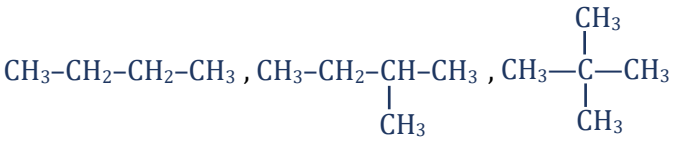
ORGANIC COMPOUND
Open–Chain, acyclic
or aliphatic compounds
Saturated
alkane
CH3–CH2–CH3
Propane
Unsaturated
alkene
CH3–CH=CH2
Propene
alkyne
HC≡CH
Ethyne
Closed–Chain or
Cyclic compound
Homocyclic
compound
Alicyclic
compounds
Cyclo
hexane
Cyclo
butene
*Aromatic
compounds
Benzene
annulene [18]
Heterocyclic
compounds
Alicyclic
compounds
O
Pentahydropyran
Aromatic
compounds
N
Pyridine
*Aromatic
compounds
Non benzenoid
(Without any Benzene ring
containing compounds)
annulene [18]
Benzenoid
(Benzene ring
containing compounds)
Benzene
Nphthalene

Classification of organic compounds :

Aliphatic or open chain compounds :

Those compounds in which first & last carbon atoms are not connected with each other. Branched or unbranched chains are possible in these compounds.

For example :



(Unbranched) (Branched)

There are two varieties in these compounds –

Saturated hydrocarbons :

(a) In such type, adjacent carbon are attached with single bonds.
Example - $CH_3–CH_2–CH_3$

(b) General formula of these compounds are C_nH_{2n+2}

(c) These are also called as paraffins (Parum + Affins i.e. little reactivity) because these are less reactive due to absence of π-bonds.

Unsaturated hydrocarbons :

(a) There will be a double bond or a triple bond between any two carbon atoms,
$CH_2 = CH – CH_3$ Propene
$CH \equiv C – CH_3$ Propyne

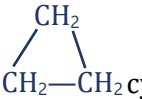
(b) General formula is C_nH_{2n} or $C_n H_{2n-2}$

(c) These are also called as olefins because they reacts with halogens to form oily substances olefins (Oleum + fines i.e. Oil forming).

(d) Due to presence of π bonds these are more reactive.

Closed chain compounds :

In these compounds first & last carbon are attached with each other.

Example  cyclopropane.

Homocyclic compounds :

These are the compounds in which the complete ring is formed by carbon atoms only. These are also of two types

(A) Alicyclic compounds : These are the compounds having the properties like aliphatic compounds. These may be saturated or unsaturated like aliphatic compounds.


cyclopropane


cyclopropene


cyclobutene

(B) Aromatic compounds : Conditions for a compound to be aromatic -

(i) Compound should be cyclic.

(ii) Compound should be planar. (All carbon in ring should be sp^2 hybridised)

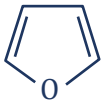
(iii) It follow Huckel's Rule :- [4n + 2] π electrons. (Odd number of π electron pairs)

n = 0	2π electrons	or 1 pair
n = 1	6π electrons	or 3 pairs
n = 2	10π electrons	or 5 pairs
n = 3	14π electrons	or 7 pairs

(iv) There should be cyclic resonance in ring.

Heterocyclic compounds :

These are cyclic compounds having ring and rings build up of more than one kind of atoms.



Furan

Thiophene

Pyrrole

Homologous Series :

A group or a series of organic compounds each containing a characteristic functional group forms a homologous series and the members of the series are called homologues. The members of a homologous series can be represented by general molecular formula and the successive members differ from each other in molecular formula by a $-CH_2$ unit. There are a number of homologous series of organic compounds. Some of these are alkanes, alkenes, alkynes, haloalkanes, alkanols, alkanals, alkanones, alkanoic acids, amines etc. It is also possible that a compound contains two or more identical or different functional groups. This gives rise to polyfunctional compounds.

Groups :

Normal groups :

(a) It is represented by 'n' :

(b) Straight chain of carbon atoms is known as normal group.

(c) Free bond will come either on Ist carbon atom or on last carbon atom.

n–propyl $CH_3–CH_2–CH_2–$

n–butyl$CH_3–CH_2–CH_2–CH_2–$

Iso group :

(a) It is represented by following structure

$CH_3–\underset{\displaystyle CH_3}{\underset{|}{CH}}–$

(b) When methyl groups are attached to the second last carbon atom, group is named as iso.

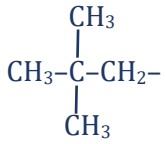
$CH_3–\underset{\displaystyle CH_3}{\underset{|}{CH}}–$ $\quad$ $CH_3–\underset{\displaystyle CH_3}{\underset{|}{CH}}–CH_2–$ $\quad$ $CH_3–\underset{\displaystyle CH_3}{\underset{|}{CH}}–CH_2–CH_2–$

Iso propyl $\quad$ Iso butyl $\quad$ Isopentyl

Neo group :

(a) When two methyl group are attached to second last carbon atom group is named neo group.

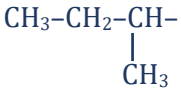
(b) It is represent by following structure -

for Ex.  Neo pentyl

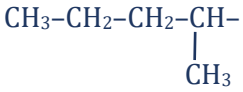
Secondary group :

(a) When two alkyl groups attached to the same carbon atom, group is named as secondary.

Ex.

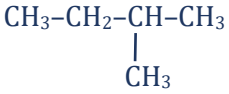


Secondary butyl



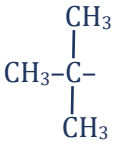
Active Secondary pentyl

(b) It is represented by following structure.

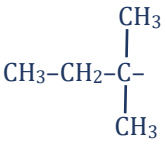


Tertiary group :

(a) When three alkyl groups (similar or dissimilar) are attached to the same carbon atom, group is name as tertiary.

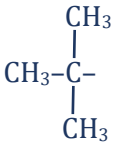


Tertiary butyl



Tertiary pentyl

(b) It is represented by following structure -

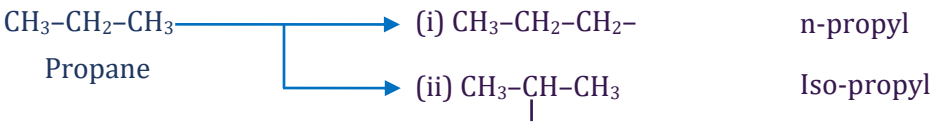


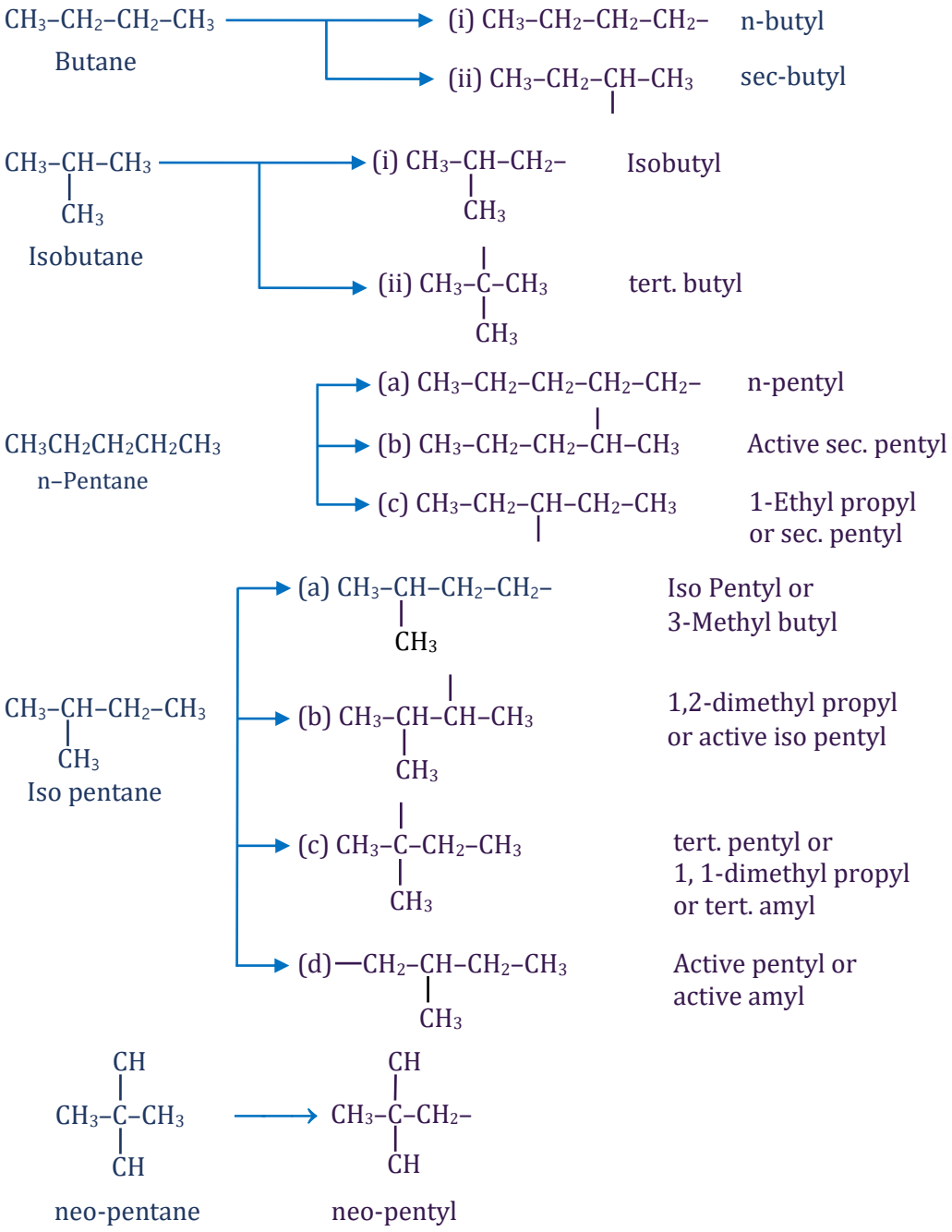
Alkyl groups :

When a hydrogen is removed from saturated hydrocarbon then alkyl group is formed. It is represented by R & its general formula is C_nH_{2n+1}. A bond is vacant on alkyl group, on which any functional group may come.

Alkane $\xrightarrow{-H}$ Alkyl (monovalent radical) $\xrightarrow{-H}$ Bivalent radical $\xrightarrow{-H}$ Trivalent radical

$CH_4 \rightarrow -CH_3$ Methyl $\qquad$ $C_2H_6 \rightarrow -C_2H_5$ Ethyl





Note 1 : Pentyl is also called amyl group.

Note 2 : (Optically active) if all valency are attached to different atoms.

(a) Alkene $\xrightarrow{-H}$ Alkenyl

Ex. $CH_2=CH_2 \longrightarrow CH_2=CH-$ Ethenyl (vinyl)

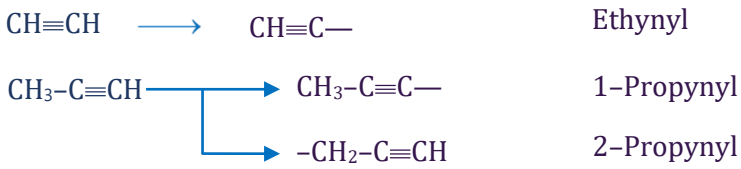
$CH_3-CH=CH_2 \longrightarrow$ (1) $CH_3-CH=CH-$ 1–propenyl

(2) $CH_3-C(CH_3)=CH_2$ Iso propenyl or 1–methyl ethenyl

(3) $-CH_2-CH=CH_2$ 2–Propenyl (Allyl)

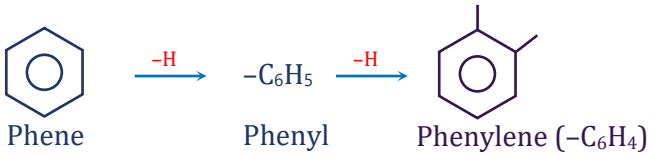
(b) Alkyne $\xrightarrow{-H}$ Alkynyl

Ex.

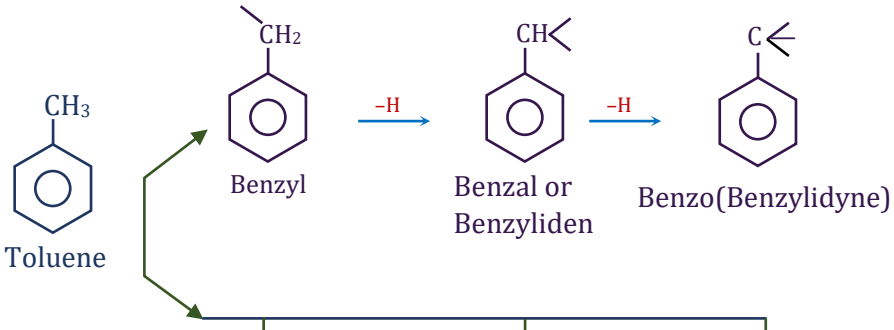


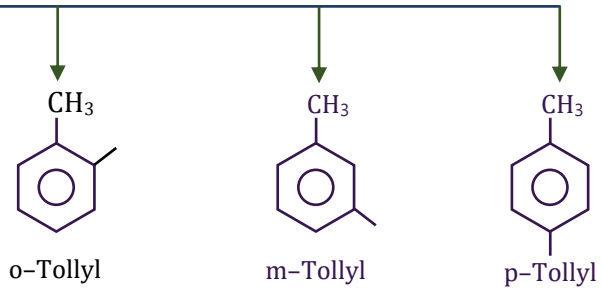
Aryl radical :

(i)

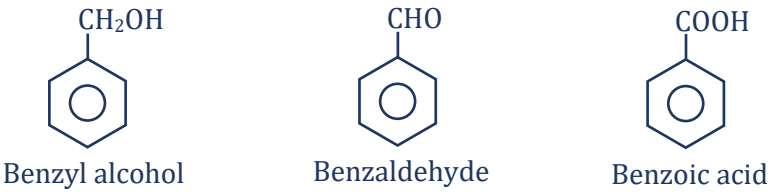


(ii)





Ex.



IUPAC system of Nomenclature :

The IUPAC system is the most widely used system of nomenclature in organic chemistry. The most important feature of this system is that any given molecular structure has only one IUPAC name and any given IUPAC name denotes only one molecular structure.

The IUPAC name of organic compound may consists of five parts, i.e.

1. Word root
2. Primary Suffix
3. Secondary Suffix
4. Primary Prefix
5. Secondary Prefix

A complete IUPAC name of an organic compound have the following sequence :

Secondary prefix +Primary prefix + Word root + Primary suffix + Secondary suffix

1. **Word root :** It is the basic unit of the name. It denotes the number of carbon atoms present in the principal chain (the longest possible continuous chain of carbon atoms including the functional group and based upon the common names of alkanes) of the organic molecules.

   Root word : According to number of carbon's in parent C–chain.

Number of carbons	Root word	Number of carbons	Root word
1	Meth	8	Oct
2	Eth	9	Non
3	Prop	10	Dec
4	But	11	Undec
5	Pent	12	Dodec
6	Hex	13	Tridec
7	Hept		

2. **Primary suffix :** A primary suffix is always added to the root word to indicate whether the carbon chain is saturated or unsaturated. The three basic primary suffixes are given below :

S. No.	Type of carbon chain	Primary Suffix	General Name
1	(a) Saturated	-ane	Alkane
2	(b) Unsaturated with one double bond	-ene	Alkene
3	(c) Unsaturated with one triple bond	-yne	Alkyne

   If the parent carbon chain contain two, three or more double or triple bond, numerical prefix such as di (for two), tri (for three), tetra (for four) etc. are added to the primary suffix. For example.

S. No.	Type of carbon chain	Primary Suffix	General Name
1	(a) Unsaturated with two double bonds	-diene	Alkadiene
2	(b) Unsaturated with two triple bonds	-diyne	Alkadiyne

3. **Secondary suffix :** A secondary suffix is always added to the primary suffix to indicate the nature of the functional group present in the organic compounds. Secondary suffix of some important functional groups are given below.

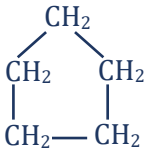
S. No.	Class of organic compounds	Functional group	Secondary Suffix
1	Alcohols	– OH	- ol
2	Aldehydes	–CHO	- al
3	Ketones	> C = O	- one
4	Carboxylic acids	– COOH	- oic acid
5	Acid amides	$–CONH_2$	- amide

6	Acid chlorides	– COX	- oyl halide
7	Esters	– COOR	alkanoate
8	Nitriles	– CN	- nitrile
9	Thioalcohols	– SH	- thiol
10	Amines	– NH_2	- amine

The following examples illustrate the use of word root, primary suffix and secondary suffix in naming of organic compounds.

S. No.	Organic Compounds	Word root	Primary suffix	Secondary suffix	IUPAC name
1	CH_3CH_2OH	Eth	an (e)	ol	Ethanol
2	$CH_3CH_2CH_2NH_2$	Prop	an (e)	Amine	Propanamine
3	$CH_3CH_2CH_2COOH$	But	an (e)	oic acid	Butanoic acid
4	CH_3CH_2CN	Prop	an(e)	nitrile	Propanenitrile
5	$CH_2 = CHCHO$	Prop	en(e)	al	Propenal
6	$HC \equiv CCOOH$	Prop	yn(e)	oic acid	Propynoic acid

4. **Primary prefix :** A primary prefix is used simply to distinguish cyclic from acyclic compounds. For example, in case of carbocyclic compounds.(cyclic compounds containing only carbon atoms in the ring.), a primary prefix, **cyclo** is used immediately before the word root. Thus.

eg. : 

Cyclo + Pent + ane = Cyclopentan

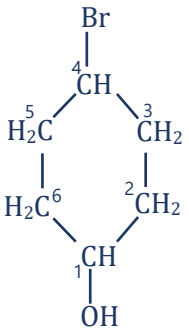
Primary + Word + Primary = IUPA

If the prefix cyclo is not used, it simply indicates that the compound is acyclic or open chain.

5. **Secondary prefix :** In IUPAC system of nomenclature, certain groups are not considered as functional groups but are treated as substituents. These are called secondary prefixes and are added immediately before the word root (or the primary prefix in case of carbocyclic compounds) in alphabetical order to denote the side chains or substituent groups. The secondary prefixes for some groups which are always treated as substituents groups (regardless of the fact whether the organic compounds is monofunctional or polyfunctional) are given below :

S. No.	Organic Compounds	Secondary prefix	Word root	Word root	IUPAC name
1	CH_3CH_2–Br	Bromo	eth	ane	Bromoethane
2	CH_3–NO_2	Nitro	meth	ane	Nitromethane
3	C_2H_5–OC_2H_5	Ethoxy	eth	ane	Ethoxyethane

In case of carbocyclic compounds, primary prefixes are also used.



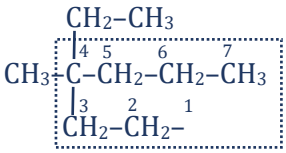
4-Bromo	+	Cyclo	+	hex	+	an (e)	+	1- ol
Secondary prefix		Primary prefix		Word root		Primary suffix		Secondary suffix

IUPAC nomenclature of branched/complex alkanes :

(1) (a) Select the longest chain of carbon atoms in the molecule.

(b) Count the number of carbon atoms in that chain and name according to the following rules.

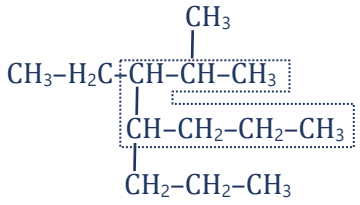
Example :



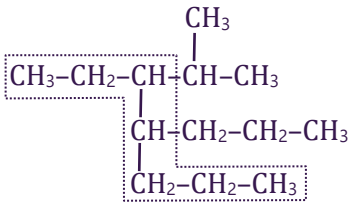
Longest chain has 7 carbons.

$\therefore$ It is a $\frac{\text{hept}}{\text{word root}} + \frac{\text{ane}}{\text{primary suffix}}$

When chains of equal lengths are competing for selection, that chain is selected which has more number of substituents.

Right 

7C in parent chain with 3 side chains

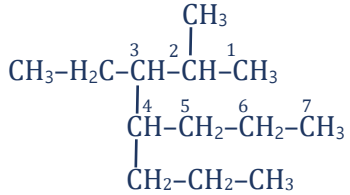
Wrong 

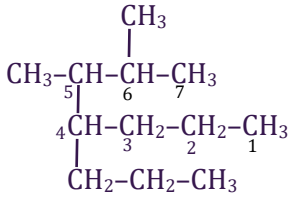
7C in parent chain with 2 side chains

Here the chain shown is selected.

(2) Carbon atoms in the longest chain selected as above in numbered consecutively form one end to the other such that the substituents attached get the lowest number.

In the above example, according to this rule, the numbering will be done as :

Right 

Wrong 

By this numbering, locant (substituents) get the number 2, 3 and 4 compared to 4, 5 and 6 if numbering is done from other end.

(3) Each substituent, which obviously, is an alkyl group is named according to number of carbon atoms present in it and it is prefixed by the number to which it is located in the main chain. In the above example, substituents are as following:

– CH_3 (methyl) group at carbon NO. 2 ⇒ 2-methyl

– C_2H_5 (ethyl) group at carbon NO. 3 ⇒ 3-ethyl

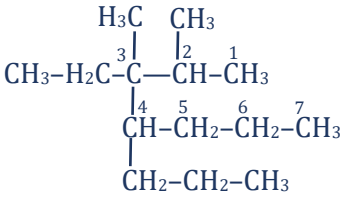
– $CH_2CH_2CH_3$ (propyl) group at carbon NO. 4 ⇒ 4-propyl

Hence, the above compound is named as : **3-Ethyl-2-methyl-4-propylheptane**

(4) If the same substituent occurs more than once in the molecule, the prefix di (for two), tri (for three), etc. used to indicate how many times it appears.

The above example can be written with a little modification as :

Example :



Methyl at No. 2, 3, Ethyl at no. 3, propyl at no.4

This will be named as : **3-Ethyl-2,3-dimethyl-4-propylheptane**

(5) The name of the compound is composed in such a manner that each substituent with its number and name is written alphabetically just before the parent's name. Prefixes di, tri, tetra etc. are not considered in deciding alphabetical order.

∴ Ethyl will be written before methyl which will be written before propyl.

Note that in the above examples, this pattern has been compiled with.

*Also, as per convention,

(i) numbers are separated each other by commas.

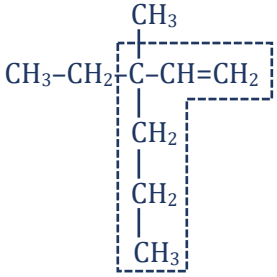
(ii) numbers are separated from words by hyphens and

(iii) write the name of the compound as a single word (with no space between)

IUPAC nomenclature of alkenes :

Functional group : –C=C–

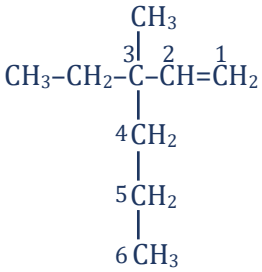
(1) Select the longest chain containing carbon-carbon double bond. This need not be the longest chain in the compound as a whole. Parent name will be alkene corresponding to number of carbon atoms in the longest chain.



Longest chain is as shown above it has 6 atoms ⇒ hexene = parent name

(2) Carbon atoms in the longest chain is numbered so that doubly bonded carbon atom gets the lowest number. The position of double bond is indicated by the smaller of the numbers assigned to two carbon atoms of double bond.

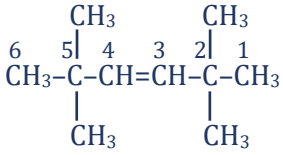
∴ The above example can be rewritten as,



Position of double bond will be indicated as no. 1.

Hence, name will be, 3-Ethyl–3–Methylhex–1–ene

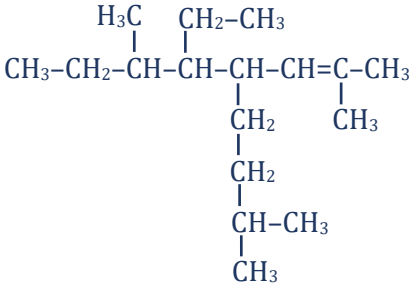
Example :



2,2,5,5–tetramethylhex–3–ene

Illustration 4:

Write the IUPAC name of the following compounds :



Solution:

5–Ethyl–2,6–dimethyl–4–(3–methylbutyl)oct–2–ene

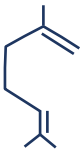
Illustration 5:

Draw the bond line structures of the following compounds.

(a) 2–Methyl–3–heptene (b) 2, 6–Dimethyl hepta –1, 5–diene

Solution:

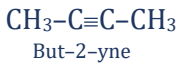
(a) 

(b) 

IUPAC nomenclature of alkynes (– C ≡ C – group) :

Numbering of longest chain is exactly same as that for naming alkenes.

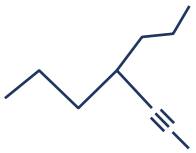
Example



But–2–yne

Illustration 6:

Write the IUPAC name of the following compounds :

(a) $CH_3-\underset{\displaystyle CH_3}{\underset{|}{CH}}-C\equiv C-CH_3$ (b) 

Solution:

(a) 4–Methyl–2–Pentyne (b) 4–Propyl–2–heptyne

Illustration 7 :

Write the IUPAC name of the following compounds :

$$H_3C-CH_2-\underset{\displaystyle H_3C}{\underset{|}{\overset{\displaystyle CH}{\overset{|}{C}}}}-\underset{\displaystyle CH_3}{\underset{|}{CH}}-C\equiv CH$$

Solution:

3, 4, 4–trimethyl–1–hexyne

IUPAC nomenclature of hydrocarbons containing both double and triple bonds occurring only once :

(i) Such hydrocarbon is named as alkenyne (not alkynene).

(ii) Numbering is done in a manner that double and triple bonds get the lowest possible number. In case of a choice, the double bond is given preference over triple bond.

Example : $CH_3-CH=CH-C\equiv CH$

5 4 3 2 1 $\Rightarrow$ multiple bonds at (1) & (3)

Note 1 2 3 4 5 $\Rightarrow$ multiple bonds at (2) & (4)

$\therefore$ Name will be Pent –3–en–1–yne

$HC\equiv C-CH_2-CH=CH_2$

5 4 3 2 1 $\Rightarrow$ Pent–1–en–4–yne

(Here there is a choice : if we number from other side)

$HC\equiv C-CH_2-CH=CH_2$

1 2 3 4 5

again multiple bonds are at numbers (1) and (4)

So, here we will give preference to double bond over triple bond.

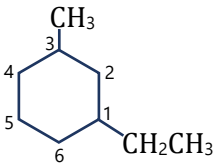
IUPAC nomenclature of alicyclic compounds :

(1) The names of alicyclic compounds are obtained by adding the prefix "cyclo"

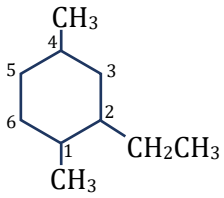
Cyclobutane Cyclopentene

(2) The numbering of the carbon atoms in the ring is done in such a way that the substituent which comes first in the alphabetical order is given the lowest possible number provided it does not violate the lowest set of locants rule

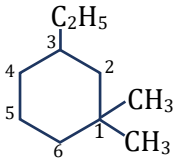
Example :



1–Ethyl–3–methyl cyclohexane



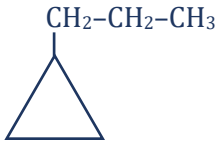
2–Ethyl–1,4–dimethyl cyclohexane



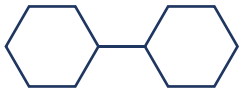
3–Ethyl–1,1–dimethyl cyclohexane

(3) When the ring contains more or equal number of carbon atoms than the alkyl group attached to it, then it is named as a derivative of cycloalkane and the alkyl group is treated as substituent

Example :



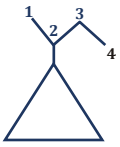
Propylcyclopropane



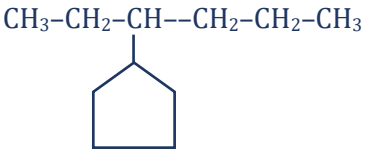
Cyclohexylcyclohexane

(4) The alkane chain contains greater number of carbon atoms than present in the ring, the compound is considered as the derivative of alkane and the ring is designated as substituent.

Example :



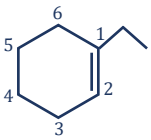
2-Cyclopropylbutane



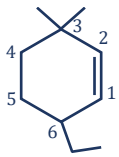
3–Cyclopentylhexane

(5) If ring has unsaturation and side chain is saturated then ring is selected as parent chain.
If side chain has unsaturation and ring is saturated then side chain is selected as parent chain.
If both have unsaturation the chain with maximum unsaturation has selected as parent chain.
If equal unsaturation then longest chain is selected as parent chain.
If unsaturation and number of carbon atoms both are equal then ring is selected as parent chain.

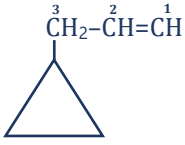
Example :



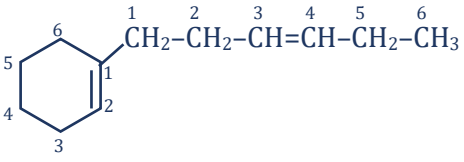
1–Ethyl Cyclohex–1–ene



6–Ethyl–3,3–dimethyl cyclohex–1–ene



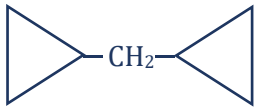
3–Cyclopropyl prop-1-ene



1-(Hex-3-ene) Cyclohex-1-ene

(6) If, more than one alicyclic ring is attached to a single chain, the compound is named as a derivative of alkane and the ring is treated as a substituent group.

Example



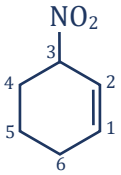
Dicyclopropylmethan

1,3-Dicyclohexyl propane

1-Cyclohexyl-4-cyclopropylbutane

(7) If a multiple bond and some other substituents are present in the ring, the numbering is done in such a way that the multiple bond gets the lowest number.

Example :

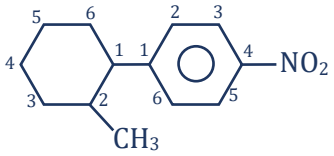


3-Nitrocyclohex-1-ene

(8) If a compound contains an alicyclic ring directly linked to the benzene ring. It is named as a derivative of benzene.

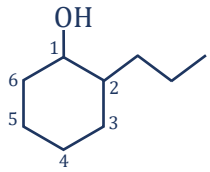
Example :

Cyclo hexyl benzene

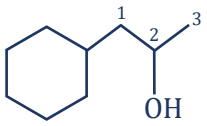


1–(2–Methylcyclohexyl)–4–nitrobenzene

(9) If functional group is present in cyclic compounds then main chain is taken where principal functional group lie, if the principal functional group is present in ring also then main chain will be taken for the maximum no. of carbon atoms.



2–propylcyclohexan–1–ol



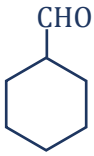
1–Cyclohexyl propan–2–ol

(10) When chain terminating functional group is directly attached with ring then ring is taken as parent chain & special suffix used for functional group.

S. No.	Functional Group	Suffix
1	—CHO	Carbaldehyde
2	—COOH	Carboxylic acid
3	—COX	Carbonyl halide
4	—COOR	Alkyl Carboxylate
5	—$CONH_2$	Carboxamide
6	—CN	Carbonitrile

Example :

Cyclohexane Carbonitrile



Cyclohexane Carbaldehyde

IUPAC nomenclature of compounds containing functional groups :

Functional Groups

Non chain terminating	Chain terminating
(i) –N=N–	(i) $-\overset{\overset{O}{\|\|}}{C}-OH$
(ii) $-\overset{\overset{O}{\|\|}}{C}-$	(ii) $-\overset{\overset{O}{\|\|}}{C}-OR$
(iii) –X	(iii) $-\overset{\overset{O}{\|\|}}{C}-X$
(iv) $-\overset{\overset{O}{\|\|}}{C}-O-\overset{\overset{O}{\|\|}}{C}-$	(iv) $-\overset{\overset{O}{\|\|}}{C}-NH_2$
(v) –O–	(v) –CN
	(vi) –CHO

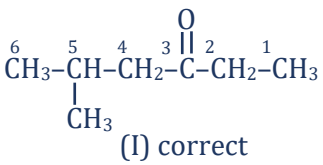
Rules for non chain terminating functional groups :

(A) Parent chain : Select the longest possible chain with maximum functional group and maximum unsaturation.

(B) Lowest number for the functional group :

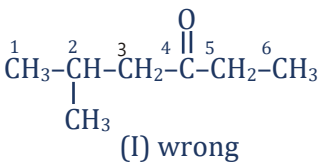
Numbering is done from that side of the chain which gives lowest locant to the principle functional group followed by double and triple bonds.

Example :



(I) correct

(> C=O group gets lowest number 3)



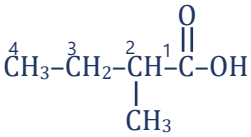
(I) wrong

(> C=O group gets number 4 which is not lowest)

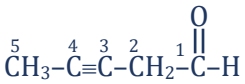
Rules for chain terminating functional groups :

(1) When a chain terminating functional group such as –CHO, –COOH, – COOR, $–CONH_2$, –COCl, – C≡N etc. is present, it is always given number 1 (one.)

Example :



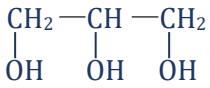
2–Methylbutan–1–oic acid



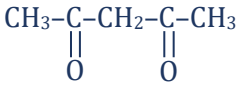
Pent-3-yn-1-al

(2) If a compound contains two or more like groups, the numerical prefixes di, tri, tetra etc. are used

Example :



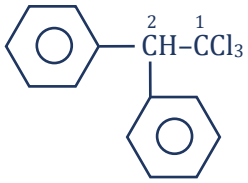
Propane –1,2,3–triol



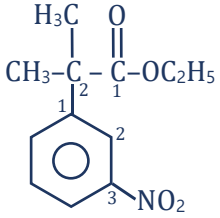
Pentane–2, 4–dione

(3) The name for benzene as substituent is phenyl. In case the phenyl ring is further substituted, the carbon atoms of the ring directly attached to the parent chain in such a ways that the substituent on the ring gets the least possible number.

Example :



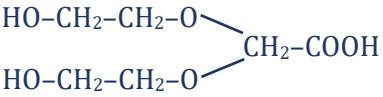
1,1,1-Trichloro-2,2-diphenyl ethane



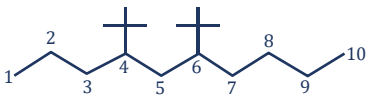
Ethyl–2–methyl–2–(3–nitrophenyl) propanoate

(4) If the organic molecule contain more than one similar complexes subtitutents, then the numerical prefixes such as di, tri, tetra etc. are replaced by bis, tris, tetrakis etc. respectively.

Example :



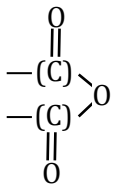
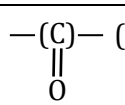
2,2–Bis–(2–hydroxyethoxy) ethanoic acid



4,6-Bis-(1,1-dimethylethyl) decane

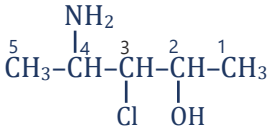
Rules for IUPAC nomenclature of polyfunctional compounds :

1. When an organic compound contains two or more different functional groups then one functional group is selected as the principal functional group while other groups are treated as substituents.

S. NO.	Functional group	Prefix	Suffix
1.	z— (C)OOH (carboxylic	×	oic acid
	— COOH	carboxy	carboxylic acid
2.	— SO_3H (sulphonic acid)	sulpho	sulphonic acid
3.	 (anhydride)	×	oic anhydride
4.	— (C)OOR (ester)	×	alkyl ------ oate
	— COOR	alkoxy carbonyl	alkyl-----carboxylate
		or carbalkoxy	
5.	— (C)OX (acid halide)	×	oyl halide
	— COX	halo formyl	carbonyl halide
6.	— (C)ONH_2 (amide)	×	amide
	— $CONH_2$	carbamoyl	carboxamide
7.	— (C)N (cyanide)	×	Nitrile
	— CN	cyano	carbonitrile
8.	— N≡C (isocyanide)	×	isonitrile
	— NC	isocyano/carbyl amino	×
9.	—CHO	formyl	carbaldehyde
10.	 (Ketone)	keto/oxo	one
11.	— OH (alcohol)	hydroxy	ol
12.	— SH (thio alcohol)	mercapto	thiol
13.	— NH_2 (amine)	amino	amine
14.	— OR (ether)	alkoxy	×

2. Some functional group such as all halo groups. (Fluoro, bromo, chloro, iodo) nitrosol, (NO) nitro (–NO_2) are always treated as substituent.

Example :



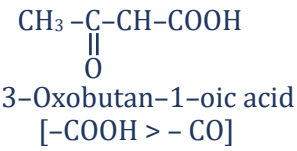
4–Amino–3–chloropentan–2–ol

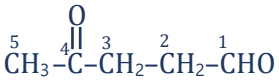
(–NH_2 & –Cl group treat as substituent)

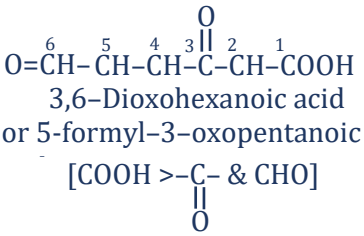
Numbering the principal chain order is

[Principal functional group > double bond > triple bond > substituents]

Example :

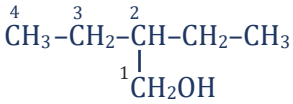

3–Oxobutan–1–oic acid
[–COOH > – CO]


4–Oxopentan–1–al
[–CHO > C=O]

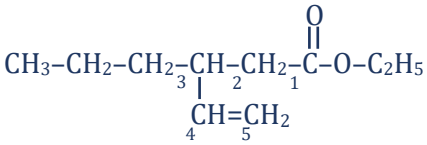

3,6–Dioxohexanoic acid
or 5-formyl–3–oxopentanoic
[COOH >–C– & CHO]

3. The longest possible chain of carbon atoms containing the principle functional group and maximum number of multiple bonds is selected as parent chain.

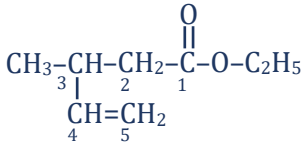
Example :

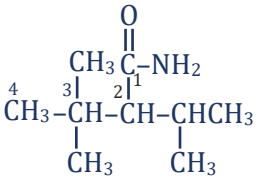
(a) 

parent chain contains four rather than five carbon atoms.

(b) 

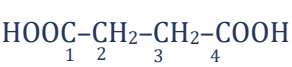
parent chain contains five rather than six carbon atoms.

(c) 
Ethyl–3–methyl–4–pentenoate

(d) 
3,3–Dimethyl–2–(1–methylethyl) butanamide

4. If more than one same chain terminating group are present then the principal chain is selected including the functional groups and numbering is done from that side which gives lowest locant to unsaturation substituent.

Example :


Butane–1,4–dioic acid

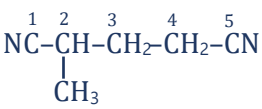
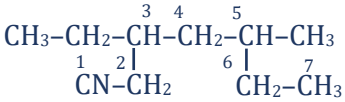

2-Methylpentanedinitrile

Illustration 8 :

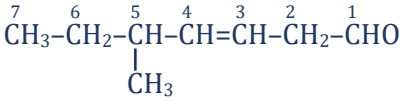
Write the IUPAC name of



1. The longest chain containing functional group is of 7 carbon atoms. Therefore, the word root is hept & the chain is numbered as shown.
2. There is no multiple bond in it. Hence, the primary suffix is ane.
3. The functional groups is –CN. Hence , secondary suffix is nitrile.
4. Moreover, there is a methyl groups on carbon 5 and ethyl group on carbon 3.
5. The IUPAC name is, therefore, **3–Ethyl–5–methylheptanenitrile**

Illustration 9:

Write the IUPAC name of



1. The longest chain containing functional group is of seven carbon atoms. Therefore, word root is hept.
2. As C=C double bond is present in the molecule. Thus, primary suffix is **ene**.
3. The secondary suffix is **al** because of presence of –CHO group.
4. The chain is numbered as shown so that carbon atoms of –CHO group gets number 1.
   The methyl group is present on carbon 5 while position of double bond is 3. Thus, IUPAC name is
   5–Methylhept–3–en–1–al

Bicyclic :

Bicyclo : When two rings are fused at two carbon then prefix Bicyclo is used.(Carbon chain should be taken in decreasing order)

(i) Two fused or bridged rings are called bicycloalkanes.

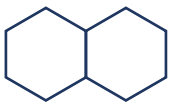
(ii) Total number of carbon atoms present in both the rings is considered as parent alkane.

(iii) Common carbon atoms present in both the rings are referred as principal points of the bridge.

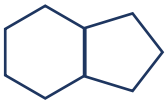
(iv) The line joining the principal points is called the bridge line. Bridge line can have 0. 1. 2 etc carbon atoms.

(v) The name is written as bicyclo [x. y. z] alkane. x. y. z are in the decreasing order.

(vi) The numbers are separated by full stops.

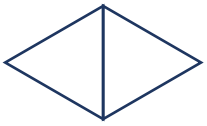


Bicyclo [4.4.0] decane

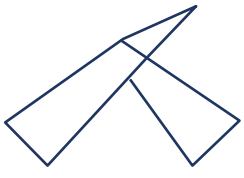


Bicyclo [4.3.0] nonane

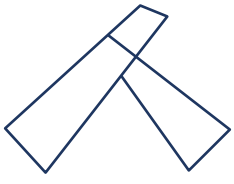
Bicyclo [2.2.0] hexane



Bicyclo [1.1.0] butane



Bicyclo [2.2.1] heptane

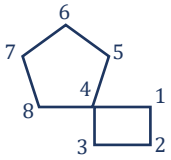


Bicyclo [2.2.2] octane

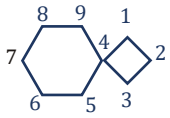
Spiro : When two rings are fused at one carbon the prefix spiro is used (Carbon chain should be taken in increasing order)

1. A molecule that has two rings sharing a single atom is called spirocyclic.
2. The numbers of skeletal atoms linked to the spiro atom are indicated by arabic numbers, separated by a full stop.
3. The numbers are written in ascending order and enclosed in square brackets.
4. Numbering of a spiro bicyclic hydrocarbon starts with a ring carbon next to the spiro atom and proceeds first through the smaller ring and then through the spiro atom and around the second ring.

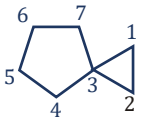
Example :



Spiro[3.4] Octan



Spiro[3.5] nonane

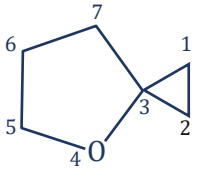


Spiro[2.4] heptane

Spiro [4.4] nonane

Spiro [2.4] heptane

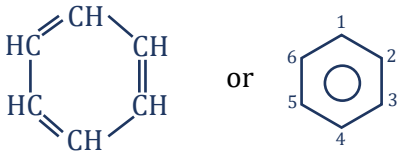
Spiro [2.2] pentane



4–oxa spiro [2.4] heptane

Nomenclature of aromatic compounds :

The aromatic compounds are cyclic compounds contains one or more benzene type rings. Benzene is the simplest hydrocarbon of aromatic series which has planar cyclic ring of six carbon atoms having three double bonds in alternate positions as shown below.



(A) Nuclear substituted –

The functional group is directly attached to benzene ring in the IUPAC system, they are named as derivative of benzene. The position of the substituents in disubstituted benzenes are indicates either by prefixes such as o–(ortho) for 1, 2, m–(meta) for 1, 3 and p (para) for 1, 4 position. However, many of their common names have also been adopted by the IUPAC system.

(B) Side–Chain substituted –

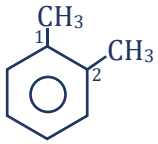
The functional group is present in the side chain of the benzene ring in the IUPAC systems, these are usually named as phenyl derivatives of the corresponding aliphatic compounds.

The IUPAC and common names of a few important members of each formly are given below :

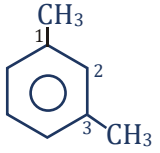
(a) Aromatic hydrocarbons (arenes) : Hydrocarbons which contain both aliphatic and aromatic units are called arenes. These are of two types

(i) Hydrocarbon containing one ring only.

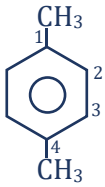
Example :



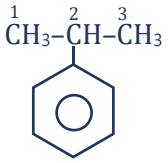
1,2–Dimethyl benzene
(o–Xylene)



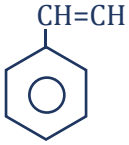
1,3–Dimethyl benzene
(m–Xylene)



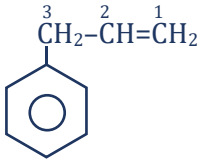
1,4–Dimethyl benzene
(p–Xylene)



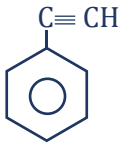
Isopropyl benzene
(Cumene)



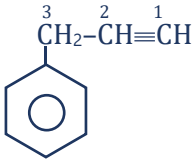
Ethenynl benzene
(Styrene)



3-propenyl benzene
(Allyl benzene)



Ethynyl benzene
(Phenyl acetylene)

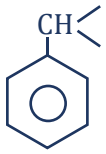


3-propynyl benzene
(Propargyl benzene)

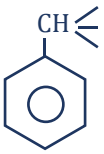
Aryl groups :


Phenyl

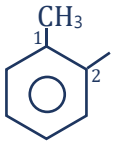
bbnbBenzyl



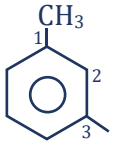
Benzal



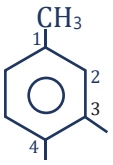
Benzo



2-Tolyl
or o-Tolyl

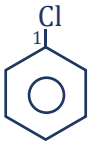


3-Tolyl
or m-Tolyl

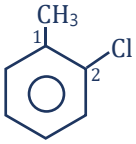


4-Tolyl
or p-Tolyl

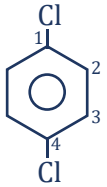
Halogen derivatives :



Chloro benzene



1,2-Dichlorobenzene
or o-Dichlorobenzene

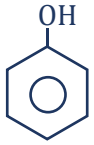


1,4-Dichlorobenzene
or p-Dichlorobenzene

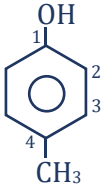
Hydroxy derivatives :

The nuclear hydroxy derivatives are called phenols while the side chain substituted hydroxy derivatives are called aromatic alcohols.

(i) Phenols–monohydric

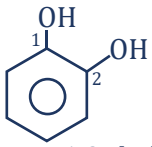


Hydroxybenzen
(phenol)

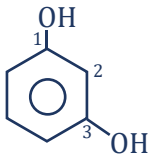


4-methyl phenol
(p-cresol)

(ii) Dihydric and polyhydric phenols



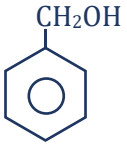
Benzene-1,2-diol
(Catechol)



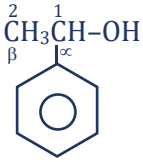
Benzene-1,3-diol
(Resorcinol)

Benzene-1,4-diol
(Quinol)

(iii) Aromatic Alcohols :

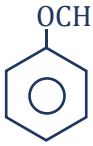


Phenyl methanol
(Benzyl alcohol)

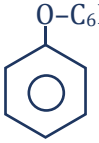


1-phenyl ethanol
(∝-phenyl ethyl alcohol)

(iv) Aromatic ethers



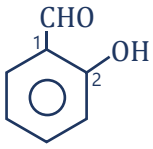
Methoxy benzene
(Anisol)



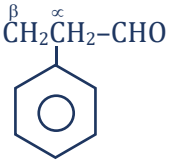
Phenoxy benzene
(Diphenyl ether)

(v) Aldehydes

Benzaldehyd

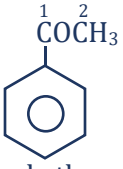


2-Hydroxy benzaldehyde
(Salicylaldehyde)

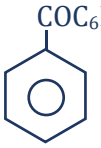


3-phenylpropanal
β-phenylpropionaldehyde

(vi) Ketones



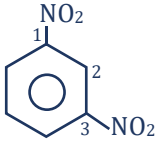
1-phenyl ethanone
(Acetophenone)



Dephenylmethanon
(Benzophenone)

(vii) Nitro Compounds

Nitrobenzene

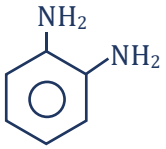


1,3-Dinitrobenzene
(m-Dinitrobenzene)

(viii) Amines

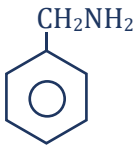
(a) Aryl amines

Benzenamin
(Aniline)

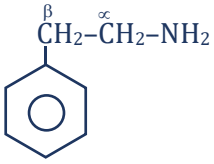


Benzene-1,2-diamine
(o-phenylenediamine)

(b) Aryl alkyl amine

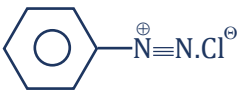


Phenyl methanamine
(Benzylamine)

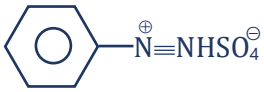


2-phenyl ethanamine
(β-phenyl ethyl amine)

(ix) Arenediazonium Salts :

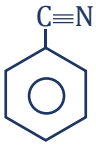


Benzene diazonium chloride

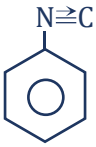


Benzene diazonium hydrogen sulphate

(x) Cyanides and Isocyanides



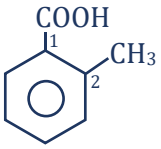
Benzonitrile
or Phenyl Cyanide



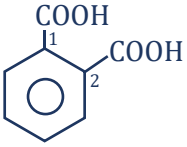
Phenyl isocyanide or
Phenyl carbylamine

(xi) Carboxylic Acids

Benzoic acid

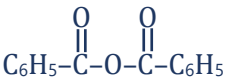


2-Methyl benzoic acid
(o-toluic acid)



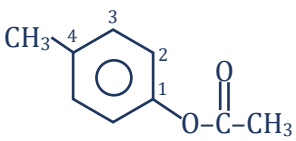
Benzene-1,2-dicarboxylic
(Pthalic acid)

(xii) Anhydrides



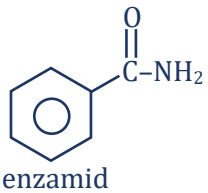
Benzoic anhydride

(xiii) Esters



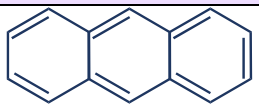
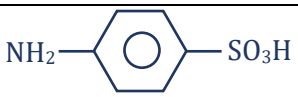
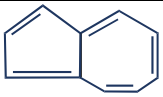
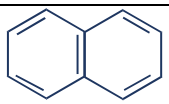
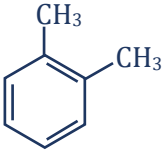
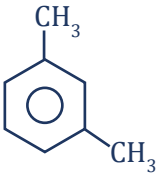
4-Methyl phenyl ethanoate

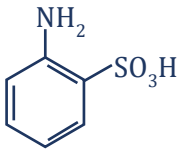
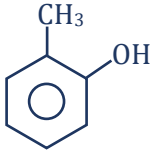
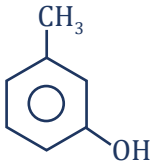
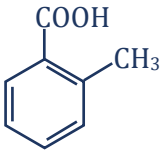
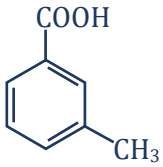
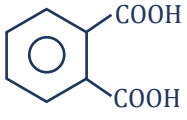
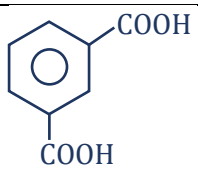
(xiv) Amides

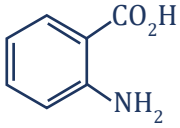
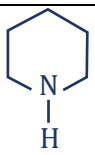
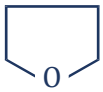
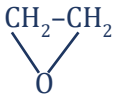
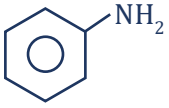
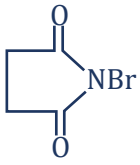


Benzamid

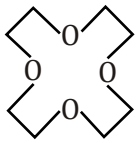
Essential common names :

ALKANE		
1.	$CH_3-\underset{\displaystyle CH_3}{\underset{\vert}{CH}}-CH_2-CH_3$	Isopentane
ALKENE		
2.	$CH_2=C=CH_2$	Allene
ALKYL HALIDE		
3.	$\underset{\displaystyle CH_3}{\underset{\vert}{CHCl_2}}$	Westron (Solvent)
4.	$ClCH=CCl_2$	Westrosol or Triclean (Solvent)
ALCOHOL		
5.	$\underset{\displaystyle CH_2-OH}{\underset{\vert}{CH-OH}}$	Glycol or Ethylene Glycol
6.	$\underset{\displaystyle OH\ \ OH\ OH}{\underset{\vert\ \ \vert\ \vert}{CH_2-CH-CH_2}}$	Glycerol
7.	$CH_2=CH-CH_2-OH$	Allyl Alcohol
8.	$CH_2=CH-OH$	Vinyl Alcohol
ETHER		
9.	$C_6H_5-O-CH_3$	Anisole (Methyl Phenyl Ether)
KETONE		
10.	CH_3COCH_3	Acetone
CARBOXYLIC ACID		
11.	$HO-\underset{\displaystyle CH_2-COOH}{\underset{\vert}{CH}}-COOH$	Malic acid
12.	$HO\ CH_2\ COOH$	Glycolic Acid
13.	$CH_2\begin{matrix}COOH\\COOH\end{matrix}$	Malonic acid
14.	$\underset{\displaystyle CH_2-COOH}{\underset{\vert}{CH_2-COOH}}$	Succinic acid
15.	$\underset{\displaystyle CH_2-COOH}{\underset{\vert}{\underset{\vert}{CH_2-COOH}}}$	Glutaric acid
16.	$CH_3-\overset{\displaystyle O}{\overset{\Vert}{C}}-CH_2-\overset{\displaystyle O}{\overset{\Vert}{C}}-O-C_2H_5$	Aceto Acetic Ester **(AAE)** or Ethyl Aceto Acetate
N–DERIVATIVES		
17.	$CH_2=CH-C\equiv N$	Vinyl Cyanide or Acrylo Nitrile
18.	$NH_2-\overset{\displaystyle O}{\overset{\Vert}{C}}-NH_2$	Guanidine
AROMATIC COMPOUNDS		
19.		Anthracene
20.		Thiophene
21.		Sulphanilic acid
22.		Azulene
23.		Napthalene
24.		o–xylene
25.		m-xylene
26.		Nitrobenzene (oil of mirbane)

27.		Orthanilic Acid
28.		o-Cresol
29.		m-Cresol
30.	$C_6H_5CO_3H$	Perbenzoic acid
31.	 o-toluic acid, m.p. 105°C  m-toluic acid, m.p. 111°C  p-toluic acid, m.p. 180°C	Toluic acids
32.		Phthalic acid
33.		Isophthalic acid

34.		Terephthalic acid
35.		Anthranilic acid (o-aminobenzoic acid)
36.	C_6H_5CHO	Benzaldehyde
HETROCYCLIC COMPOUNDS		
37.		Pyrrolidine
38.		Piperidine
39.		Tetrahydrofuran (THF)
40.		Oxirane or Ethylene Oxide or Oxo Cyclo Propane
41.		Quinuclidine
42.		Aniline
SOME REAGENTS		
43.	Grignard's reagent	RMgX
44.	NBS 	N-Bromosuccinimide
POLAR PROTIC SOLVENTS		
45.	H –O–H	Water
46.	R–O–H	Alcohol

47.		Phenol
48.	$CH_3-\underset{\underset{O}{\|}}{C}-OH$	Acetic acid
49.	HF	Hydrogen Fluoride
Polar Aprotic Solvents		
50.	DMS	Dimethyl sulphide CH_3-S-CH_3
51.	DMSO	Dimethylsulphoxide $Me_2S=O$

52.	HMPT or HMPTA	Hexamethylphosphoramide $O=P-(NMe_2)_3$
53.	DMF	Dimethyl formamide $H-\underset{\underset{O}{\|}}{C}-NMe_2$
54.	Crown ethers  (12 – C – 4)	Cyclic polyethers
55.	NH_3	Ammonia