NOMENCLATURE OF ORGANIC COMPOUND

Classification of organic compounds

Organic compounds are broadly classified into following to classes

1) Acyclic compounds

These are the compounds in which carbon atoms are linked to form open chain (straight or branched). These compounds may be saturated(all single bonds) or unsaturated (multiple bonds)

Example

Propane $CH_3 – CH_2 – CH_3$ is saturated as it contains single bond between two carbon atoms

Propyne $CH_3 – CH = CH_2$ is unsaturated as it contains double between tow carbon atoms

2)Cyclic compounds/ close chain/ ring compounds

These are the compounds which contains one or more closed ring in their molecule. These are further of two types

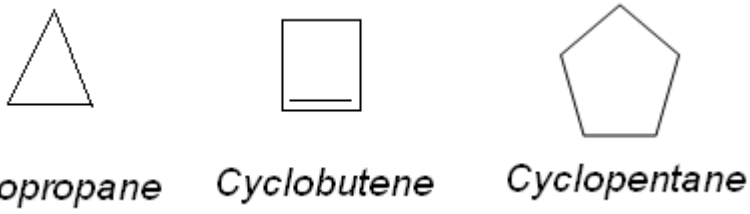
(a) Homocylic compounds

These are the cyclic compounds in which ring is made of only one type of atoms. These are further divided into two sub-classes

These are the cyclic compounds in which ring is made of only one type of atoms. These are further divided into two sub-classes

(i)Alicyclic compounds

These are the carbocylic compounds which resemble corresponding acyclic compounds in their properties e.g.

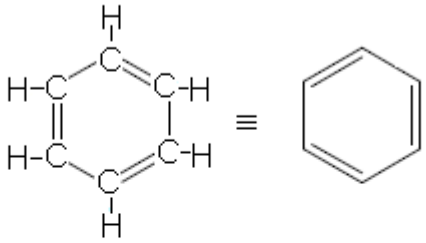


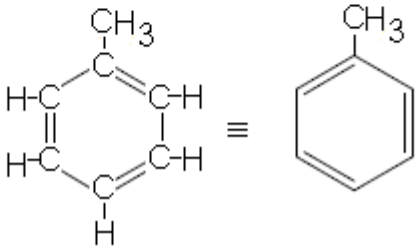
Cyclopropane *Cyclobutene* *Cyclopentane*

(ii)Aromatic homocyclic compounds

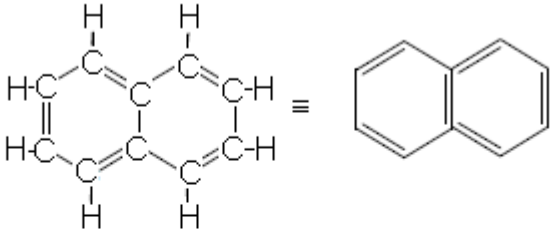
These are the compounds which contains one or more fused or isolated benzene ring. These are also called benzenoid compounds e.g.

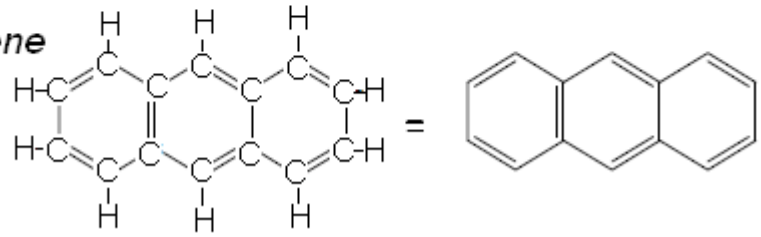
Monocyclic

benzene 

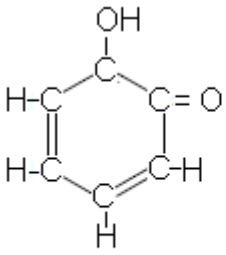
toluene 

Polycyclic

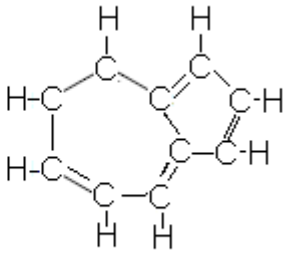
naphthalene 

anthracene 

There are some other aromatic homocyclic compounds which do not contain benzene ring. Such compounds are known as non-benzenoid compound



Tropolone



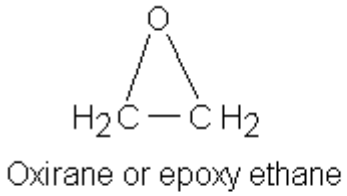
Azulene

(b)Heterocyclic compounds

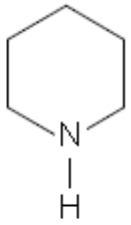
These are the cyclic compounds which contains one or more heteroatoms (atoms other than C and H) in the ring. These are further divided into two subclasses

(i)Alicyclic heterocyclic compounds

The heterocyclic compounds which resemble the corresponding aliphatic compound in most of the property is known as alicyclic heterocyclic compounds examples



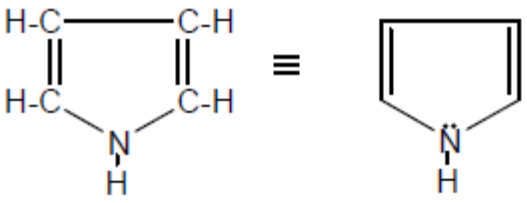
Oxirane or epoxy ethane



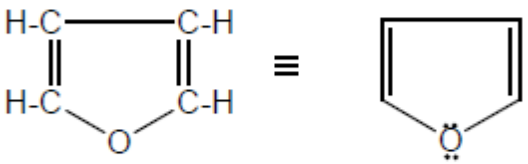
Piperidine

(ii) Aromatic heterocyclic compounds

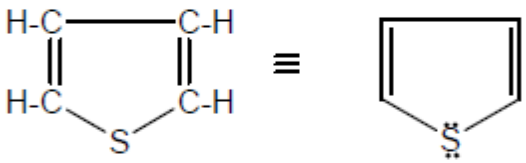
These are the heterocyclic compounds which posses aromaticity and resemble corresponding aromatic compounds in most of their property. These are also called non-benzenoid aromatic compounds. Examples



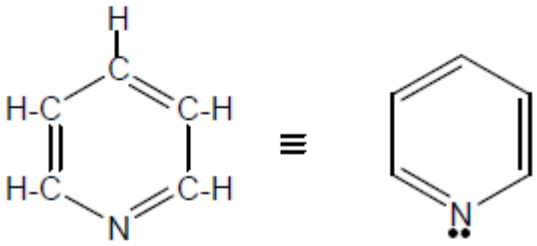
pyrrole



furan



thiophene



pyridine

Homologous series

It is a series of compounds in which the adjacent members differ by a $–CH_2-$ unit. All the members of such a series have same general formula, same functional group, same chemical properties and show regular gradation in physical properties e.g. members of homologous series of alkenes have general formula C_nH_{2n},

Two successive members differ by $–CH_2-$ unit. Individual members of such series are called homologues and the phenomenon is called as homology.

Functional group

It is an atom or group of atoms that decides the chemical nature of an organic compound . For example -OH (hydroxyl), $-NH_3$(amine) etc

NOMENCALATURE OF ORGANIC COMPOUND

The world wide accepted system for naming organic compounds is IUPAC system of nomenclature (International Union of Pure and Applied Chemistry) according to which all organic compounds are considered as derivative of saturated hydrocarbons. The IUPAC name of an organic compounds consists of three parts: word –root, suffix and prefix

(i)Word root

Word root gives the idea about principle carbon chain. Word root is given according to number of carbon atoms in a carbon chain

Number of carbons	Word root	Number of carbon	Word root
1	Meth-	7	Hept-
2	Eth-	8	Oct-
3	Prop-	9	Non-
4	But-	10	Dec-
5	Pent-	11	Undec
6	Hex-	12	Dodec-

(ii)Suffix

There are two type of suffixes

(a)Primary suffix

It gives the idea about saturation and un-saturation of the organic compound. It is always added to the word root. Primary suffix for various saturated and unsaturated carbon chains as follows

Type of carbon chain	Suffix	IUPAC
Saturated, C – C	-ane	Alkane
Unsaturated, C = C	-ene	Alkene
Unsaturated, C≡C	-yne	Alkyne

If the parent chain contains two or more multiple bonds then numerical prefixes such as di (for two), tri (for three), tetra (for four) etc. are added to the primary suffix

Examples

Organic compound	Word root	Primary suffix	IUPAC name
$CH_2CH_2CH_3$	Prop	ane	Propane
$CH_2 = CH_2$	Eth	ene	Ethane
$CH_3C{\equiv}CH$	Prop	yne	Propyne
$CH_2 = CH - CH = CH_2$	But	dine	Butadiene

(b) Secondary suffix

Secondary suffix gives the idea about nature of the functional group present in the compound. It is added after primary suffix. Secondary suffix for some common functional groups are as follows

Class of compounds	Functional group	Secondary suffix
Alcohols	-OH	-ol
Aldehydes	-CHO	-al
Ketones	>C = O	-one
Carboxylic acids	-COOH	-oic acid
Acid amides	$-CONH_2$	-amide
Acid chloride	-COCl	-oyl chloride
Esters	-COOR	-oate
Nitriles	-CN	-nitrile
Amine	$-NH_2$	-amine
Thioalcohol	-SH	-thiol
Sulphonic acid	$-SO_3H$	-sulphonic acid

Examples

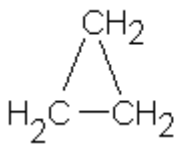
Organic compound	Word root	Primary suffix	Secondary suffix	IUPAC name
$HC{\equiv}C\text{-}CHO$	Prop	yne	Al	Propynal
$CH_3CH_2CH_2CN$	But	ane	Nitrile	Butane nitrile
CH_2 =CHOH	Eth	ene	ol	Ethenol
CH_3CH_2COOH	Prop	ane	Oic acid	Propanoic acid

(iii)Prefix

Prefixes are of two types

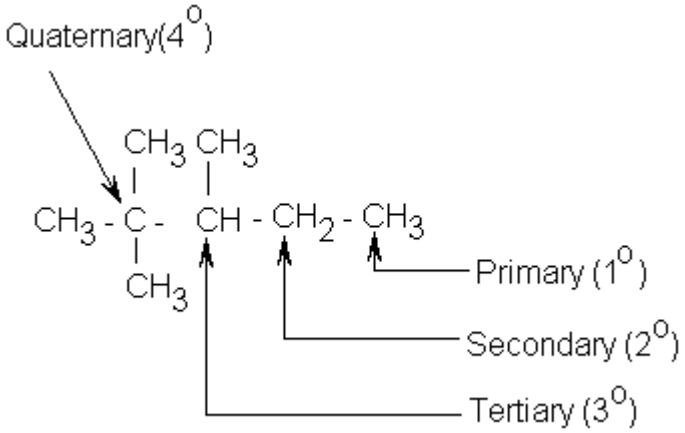
(a)Primary prefix

Primary prefix is used to give idea about cyclic or acyclic nature of the compound. For carbocyclic compounds a primary prefix cyclo is added before word root whereas in case of acyclic compounds no prefix is used Example



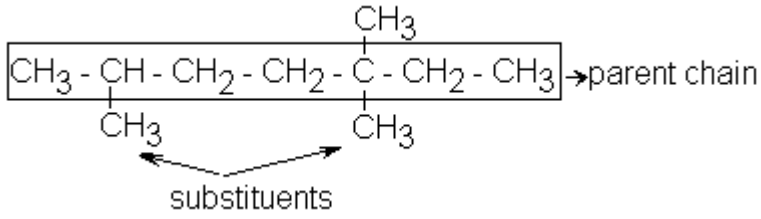
Cyclo + Prop + ane = Cyclopropane

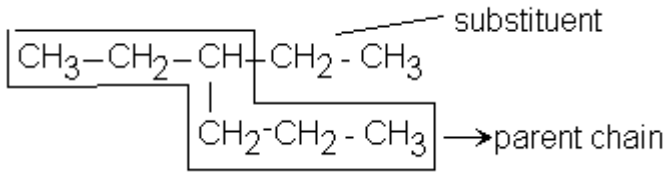
Types of carbon atoms
(i)Primary or 1^O carbon atom
A carbon atom attached to one (or no) other carbon atom
(ii)Secondary or 2^O carbon atom
It is the carbon atom attached to two other carbon atoms
(iii)Tertiary or 3^Ocarbon atom
It is the carbon atom attached to three other carbon atoms
(iv)Quaternary or 4^O carbon atom
It is the carbon atom attached to four other carbon atoms



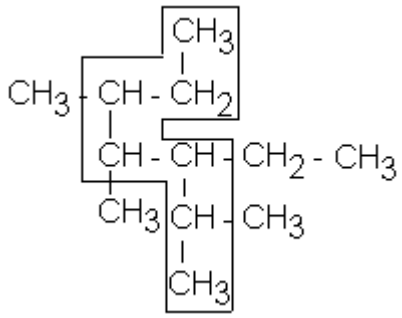
Hydrogen atom attached to 1^o, 2^o, 3^o carbon atoms are called primary (1^o), secondary (2^o) and tertiary(3-o_) hydrogen atoms respectively.

Rules for nomenclature of organic compounds
1.Longest chain rule
(i)Select the longest continuous chain of carbon atoms in the molecules. The longest continuous chain, containing the maximum number of carbon atoms, is taken as the parent chain and other part which are not included in parent chain are identified by substituents or branched chain

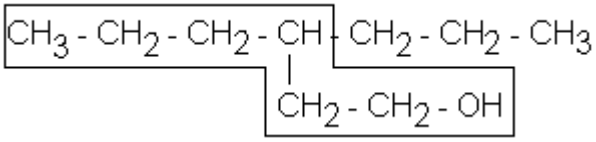




(ii) If two different chain of equal lengths are possible, the chain with maximum number of side chains of alkyl group is selected

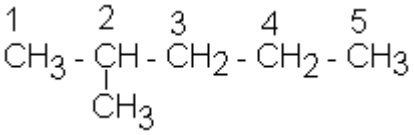


(iii) If the compound contains one functional group or multiple bonds or substituent then select the longest chain of carbon atoms containing functional group and maximum number of multiple bonds as parent chain

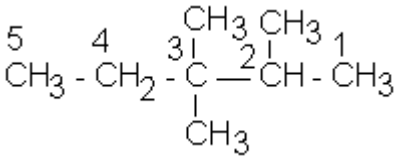


2.Numbering of the principal chain

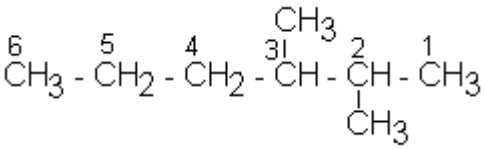
(i)Number the carbon atoms in the parent chain as 1,2,3. ….etc starting from end which gives smaller number to the carbon atoms carrying the substituent



(ii) When the parent chain has two or more substituent's, numbering should be done in such a way that sum of locants on the parent chain is lowest possible number.



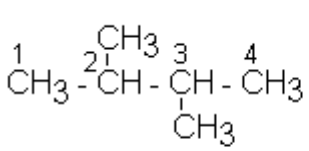
Set of locant = 2, 3, 3 (2+3+3 =8)



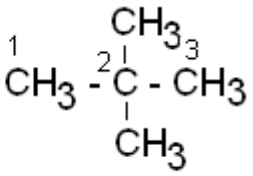
Set of locants = 2, 3 (2+3 = 5)

3. Presence of more than one same substituent

If the same substituent occurs more than once on the parent chain, it is indicated by the prefixes such as di, tri, tetra, etc to 2, 3, 4 etc. same substituent



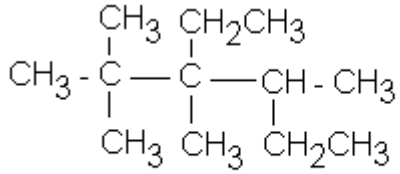
2, 3 - Dimethylbutane



2,2 -Dimethylpropane

4.Naming different substituent

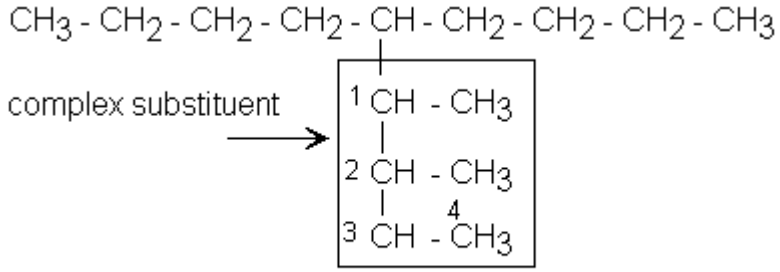
If two or more substituent are present on the parent chain, they are named in the alphabetical order along with their appropriate position



3, 4 - Diethyl - 2, 2, 4 - Trimethyl pentane

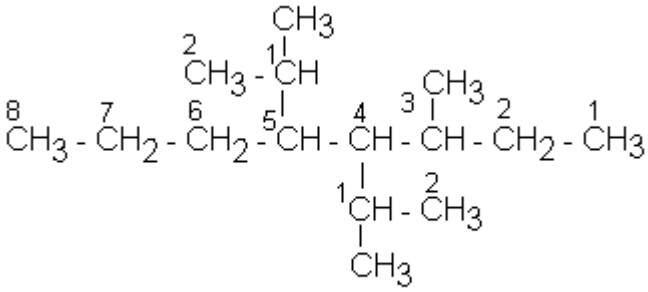
5.Naming the complex substituent

If the substituent on the parent chain is complex (i.e. it is branched) it is named as a substituted alkyl group by numbering the carbon atom of this group attached to the parent chain as 1. The name of such substituent is written in bracket in order to avoid any confusion with the numbering of the parent chain



Complex substituent : 1,2 - Dimethyl propyl

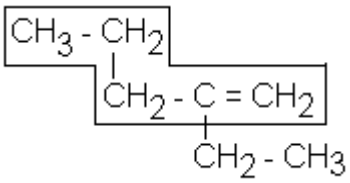
If the same complex substituent is repeated twice or thrice in the compound then prefixes bis(for two), tris (for three), tetrakis (for four) etc. are used before the name of complex substituent



3 - Methyl - 4,5 - bis(1-methyl ethyl) octane

6.Nomenclature of unsaturated hydrocarbons (Containing double or triple bond)

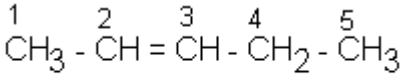
i)Select the longest continuous chain containing the carbon atom involved in the multiple bonds



ii) While writing the name of the alkene or alkyne, the suffix 'ane' of the corresponding alkane is replaced by 'ene' or 'yne ' respectively

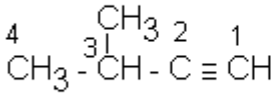
iii)IF the multiple bond occurs twice in the parent chain the alkene and alkyne are called diene and diyne respectively

iv) The numbering of atoms in parent chain is done in such a way that the carbon atom containing the double or triple bond gets the lowest number

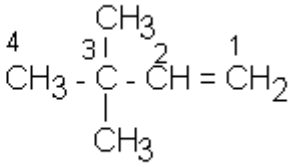


Pent - 2 - ene

v) All the rules for naming the side chains or substituent are then follows



3 -methyl but - 1 - yne

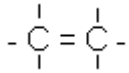


3, 3 - Dimethyl but - 1 - ene

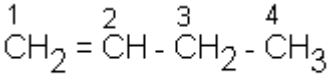
7. Functional group and their nomenclature

i)Alkene

Functional group



Replace ane of alkane by ene

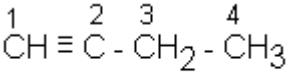


But - 1 - ene

ii)Alkyne

- C ≡ C –

Replace ane of alkane by yne

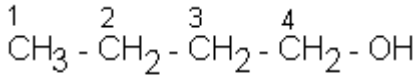


But - 1 - yne

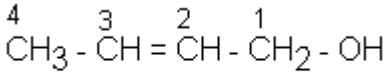
iii)Alcohol

- OH

Relace e of alkane by 'ol'



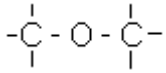
Butan -1 -ol



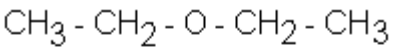
But - 2 -en - 1 -ol

Note : if parental chain contain single bond, double bond or triple bond then 'e' from ane, ene or yne will be dropped only if it is followed by 'a', 'i' 'o', 'u' , 'y'

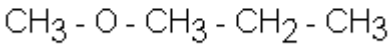
iv)Ether



These are written as alkoxy alkanes, if chain is unsymmetric then '-oxy' is attached to lower carbon chain



Ethoxy ethane



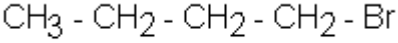
methoxy propane

v) Alkyl halides

F , Cl, Br, I

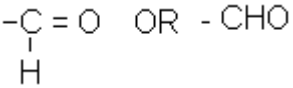
Prefix fluoro, chloro, bromo, iodo is used for F, Cl, Br and I respectively

These are named as haloalkanes

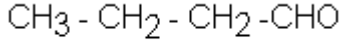


1 - Bromobutane

vi) Aldehydes

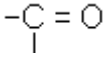


Replace 'e' of alkane by –al

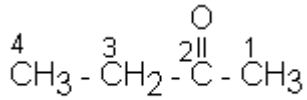


Butanal

vi)Ketones

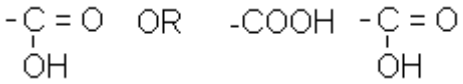


Replace 'e' of alkane by one

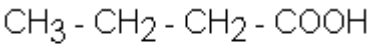


But - 2 - one

vii)Caboxylic acid

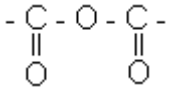


Replace e of alkane by –oic acid

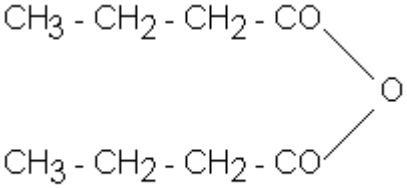


Butanoic acid

viii) Acid anhydride

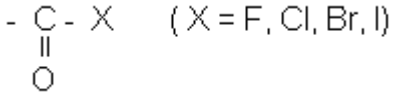


Replace ‘e’ of alkane by oic anhydride

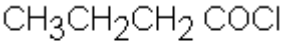


Butanoic anhydride

ix) Acid halide

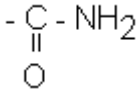


Replace oic acid of corresponding acid by oyl halide

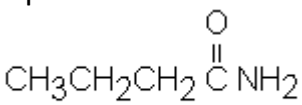


Butanoyl chloride

x) Amide

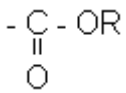


Replace oic acid of corresponding acid by amide

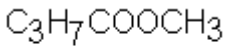


Butamide

xi)Ester



Naming the alkyl group (R) and change oic acid of acid by one



methyl butanoate

xii)Nitro

- NO_2

Naming as nitroalkane

$CH_3CH_2CH_2CH_2NO_2$

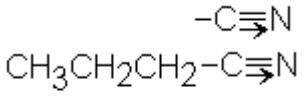
1 -nitrobutane

xiii) Nitride

- C≡N

CH_3CH_2 $CH_2C \equiv N$ Butanenitride or cyanopropane (Note if cyano is used Carbon with nitrogen is not counted)

xiv) carbylamines



Propane carbylamine

xv) Amine

- NH_2

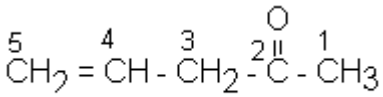
$CH_3CH_2CH_2CH_2 – NH_3$

1 – Butanamine

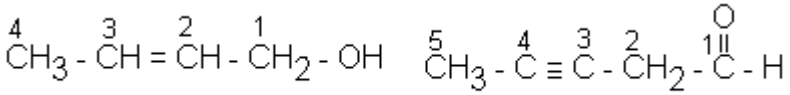
8.Nomenclature of compounds having functional groups, multiple bonds, side chains/ substituent

(i)If the organic compounds contains a functional group, multiple bond, side chain or substituent, the order of preference is

Functional group > Double bond > Triple bond > substituent

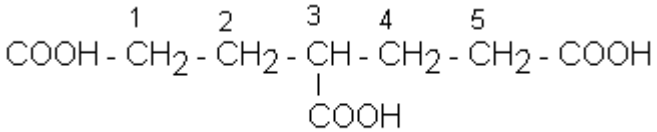


Pent - 4 - en - 2 -one



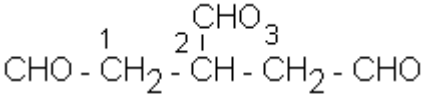
But - 2 - en - 1 - ol Pent - 3 - yn - al

9. Compound containing more than two like functional groups



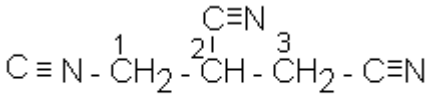
Pentane - 1,3,5 - tricarboxylic acid

Note : since word carb used carbon in functional group –COOH is not counted



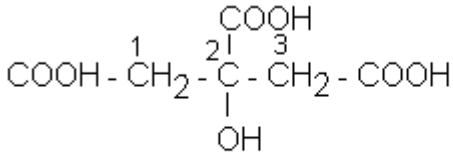
Propane - 1,2,3 tricarbaldehyde

Note : since word carb

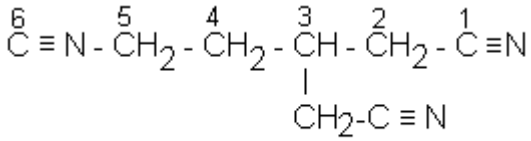


Propane - 1,2,3 - tricarbonitride

Note : since word carb is used carbon in functional group –C≡N is not counted

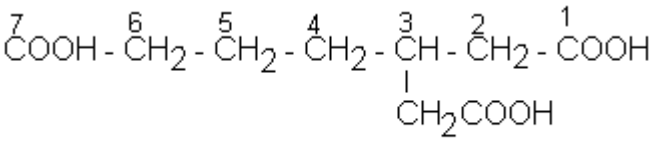


2 - Hydroxy propane - 1, 2, 3 - tri-carboxylic acid



3 - (cyanomethyl) heptane - 1,7 dioic acid

Note : since carb word is not used carbon in C≡N is also counted



3 - (carboxy methyl) heheptane - 1,7 dioic acid

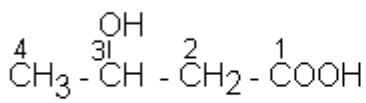
10. Nomenclature of poly – functional organic compounds

When an organic compound contains two or more functional groups, one group is treated as principal functional group and other group is regarded as the secondary functional group and may be treated as substituent

The order of for the preference of principal functional group is given below

Carboxylic acid > sulphonic acid > anhydrides> esters > acid chloride > acid amides > nitriles > aldehydes > ketones> alcohols> phenol > thiols > amine > ethers > alkene > alkynes > halo , nitro, alkyl

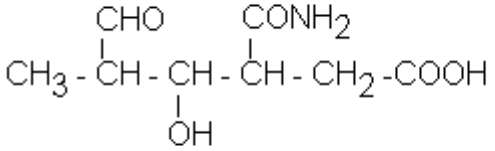
All other functional groups halo (fluoro, chloro, bromo, iodo) nitro (-NO_2), nitroso (- NO) and alkoxy (-OR) are always treated as substituent groups



-COOH is principal functional group

- OH is substituent

3 - Hydroxybutan - 1 -oic acid



-COOH is principal functional group

-CHO, -OH, -CONH2 are substituent group

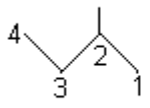
3 -carbamoyl - 5 - formyl - 4 - hydroxyhexan - 1 - oic acid

The names of secondary groups which are used as prefixes are given below

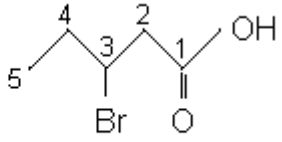
- COOH : Carboxy
-COOR : Alkoxy carbonyl or carbalkoxy
-COCl : Chloroformyl
-$CONH_2$: Carbamoyl
-CN : Cyano
-OR : R –oxy
-SO_3H : Sulpho
-CHO : Formyl
>CO : Oxo or keto
-OH : Hydroxy
-SH : mercapto
-NH_2 : amino
=NH : Imino
R-CH = CH – :alkenyl
R – C ≡ C - : Alkynyl

11. Bond line notations

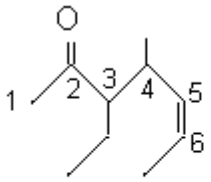
In this type of structural formulas, carbon-carbon bond is represented by a line drawn in zig-zig fashion, in which the line ends and intersections represents the carbon atom. A single bond is represented, by a single line (-) , a double bond by two parallel lines (=)and triple bond by three parallel lines (≡). Carbon and hydrogen atoms are not shown on a bond line structural formula but other atoms are shown by their usual symbols



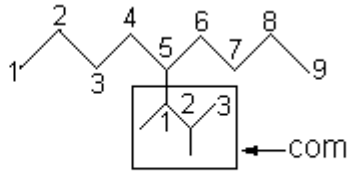
2-methyl butane



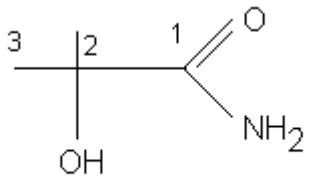
3 - bromopentan-1-oic acid



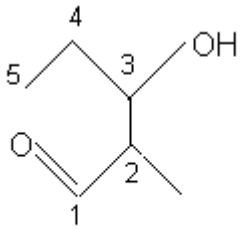
3-ethyl-4,methyl hept -5-ene-2-one



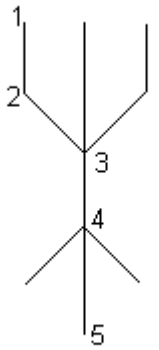
5-(1,2 - dimethyl propyl) nonane



2-Hydroxy - 2- methyl propanamide



3-Hydroxy-2-methylpentan-1-al

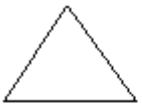


3 -ethyl - 3,4,4 trimethylpentane

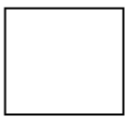
12. Nomenclature of alicyclic compounds

Following rules are generally followed for naming of alicyclic compounds

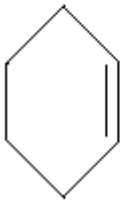
i) In the naming of such compound a prefix cyclo is added to the word root



Cyclopropane

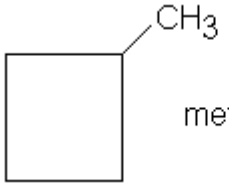


Cyclobutane



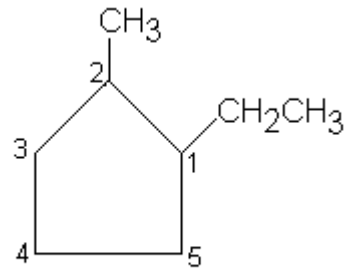
Cyclohexene

ii) If only one substituent is present on the ring, then it is not required to give its position

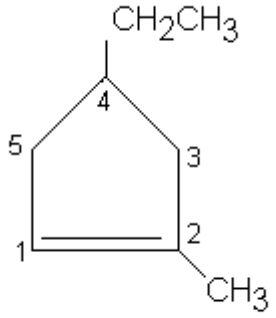


methyl cyclo butane

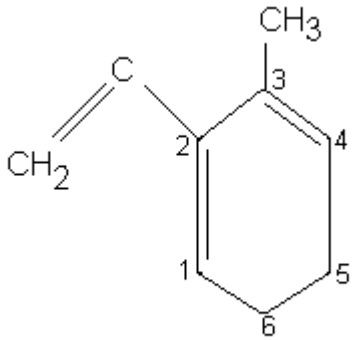
If two or more substituent are present in the ring, their positions is done by numbering of ring according to lowest set of locants rule



1 - ethyl - 2 - methylcyclopentane

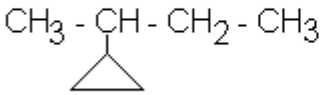


4-ethyl-2-methyl cyclopent-1-ene

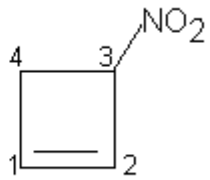


2-ethyl-3-methylcyclohexa-1,3-deine

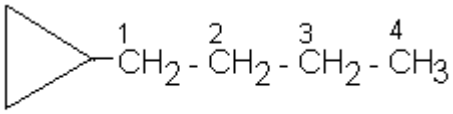
iii) If the ring contains lesser number of carbon atoms than that of alkyl group attached to it, the compound is named as derivative of alkane and the ring is considered as a substituent group to the alkane, otherwise it is named as derivative of cycloalkane.



2 - cyclopropylbutane

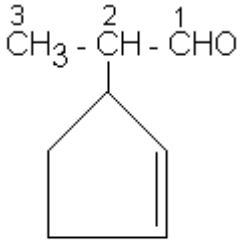


3 - nitrocyclobut-1-ene

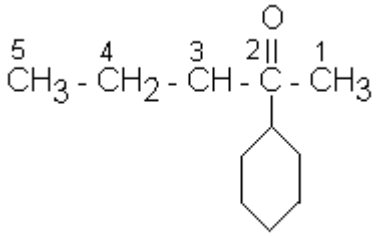


1 - cyclopropyl butane

iv) If the side chain contains a multiple bond or a functional group, then alicyclic ring is treated as the substituent irrespective of the size of the ring and/ or alicyclic ring contains multiple bonds or not

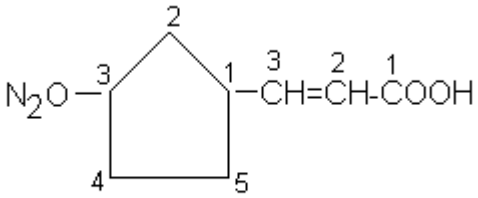


2 -cyclopentyl propanal

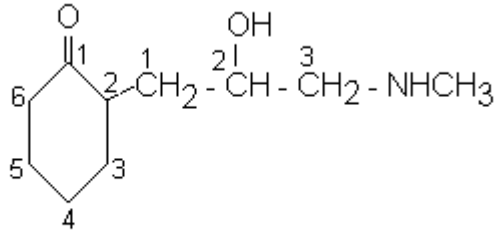


3 - cyclohexyl pentan - 2 -one

v) if both the rings as well as side chain contain the functional group, then parent hydrocarbon is then parent hydrocarbon is decided on the basis of principal functional group which is further based on preferential order of functional groups

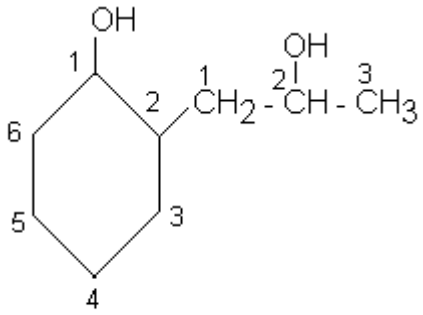


3 - (3 - Nitrocyclopentyl) prop - 2 - en - 1 - oic acid

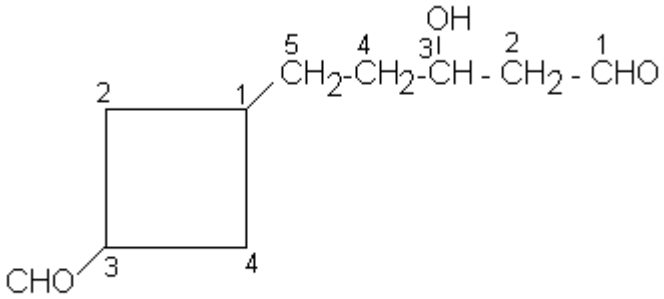


2 - (3 aminomethyl - 2 - hydroxypropyl) cyclohexan - 1 - one

vi) If both alicyclic ring and the side chain contains same functional group, the parent hydro-carbon is selected on the basis of number of carbon – atoms in the ring and side chain

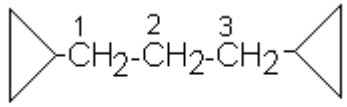


2 - (2-Hydroxypropyl) cyclohexane - 1 - ol

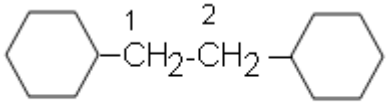


5-(3-formylcyclobutyl)-3-methyl pentanal

vii) If more than one alicyclic rings are attached to the single chain of carbon atom, the compound is named as a derivative of alkane and alicyclic rings are treated as substituent irrespective of the number of carbon atoms in the ring or chain

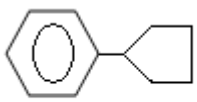


1, 3 - dicyclopropyl propane

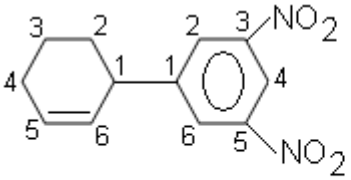


1, 2 - dicyclohexylethane

viii)If the alicyclic ring is attached to the benzene ring, the compound is named as a derivative of the benzene

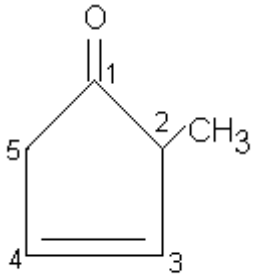


Cyclopentyl benzene

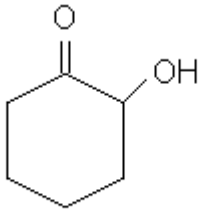


1-(2-methylcyclohex-2-ene-1-yl)-3,5-dinitrobenzene

ix) If the alicyclic ring has a functional group along with some substituent on the ring, then appropriate prefixes and suffix are used and numbering is done in such a way that the functional group gets the lowest possible number

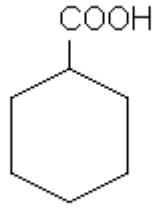


2 - methyl cyclopent-3-en-1- one

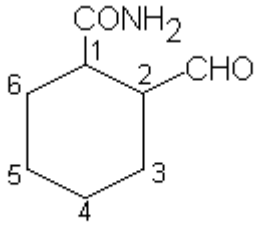


3-amino - 2-hydroxycyclohexan-1-one

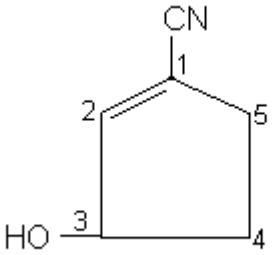
x) If an alicyclic ring is directly attached to a carbon, containing functional group, the carbon – atom of the functional group is not counted for word root rather appropriate suffix (use carb-) are used to represent such group.



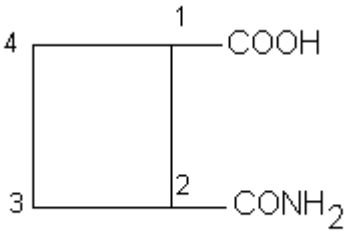
Cyclohexanecarboxylic acid



2-Formyl cyclohexane - 1 - carboamide



3-hydroxy cyclopent-1-en-1-carbonitrile



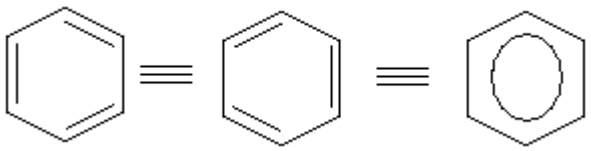
2-carbamoyl cyclobutane-1-carboxylic acid

13.Nomenclature of aromatic compounds

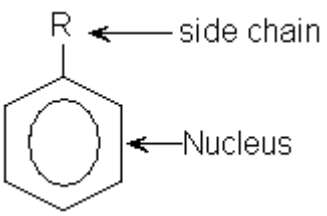
An aromatic compound consists of two parts i.e. nucleus and side chain

(a)Nucleus

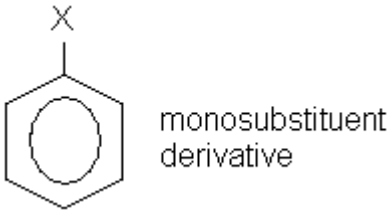
The benzene ring present in aromatic compound is called nucleus. It is represented as follows



(b) side chain



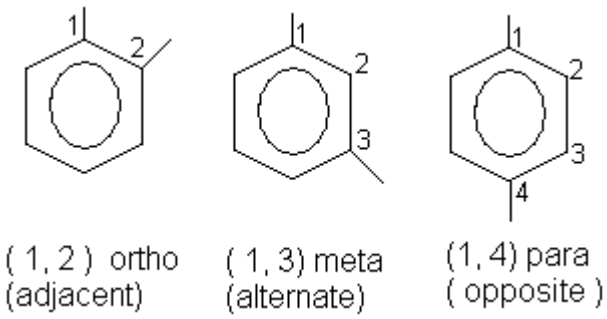
Alkyl or any other aliphatic group attached to benzene nucleus by replacing one or more hydrogen



monosubstituent derivative

If only one hydrogen atom of ring is replaced by some other group, then it is called as mono substitute derivative

If more than one hydrogen atom of benzene ring is replaced by some other atom or group, then their position is mentioned by numbering,. In +++++case of distribution respective position of two groups can also be mentioned as follows

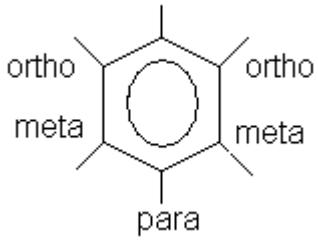


(1, 2) ortho (adjacent)

(1, 3) meta (alternate)

(1, 4) para (opposite)

With respect to a particular group the three positions can be represented as



Aromatic compounds are basically of two types

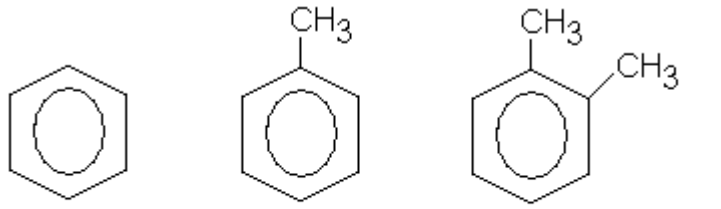
i) Nuclear substituted aromatic compounds

These are the compounds in which functional group is directly attached to benzene ring are named as derivative of benzene

ii)Side chain substitute aromatic compounds

these are the compounds in which functional group is present in the side chain of the benzene ring. These are named as phenyl derivatives of the corresponding aliphatic compounds

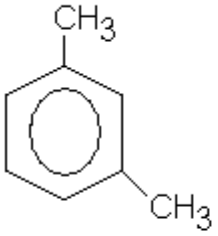
(A)Aromatic compounds



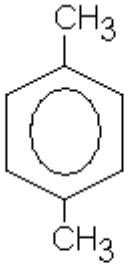
Benzene

Toluene

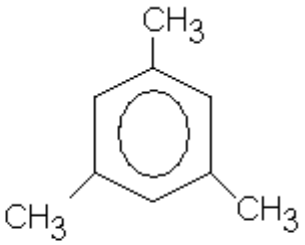
1,2 - dimethyl benzene (o- xylene)



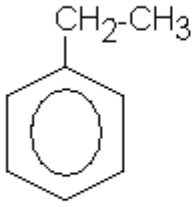
1, 3 - Dimethyl benzene
(m-xylene)



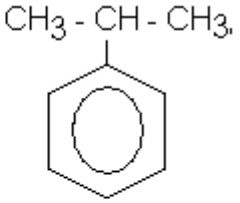
1, 4 - Dimethyl benzene
(p -xylene)



1, 3, 5 - trimethyl benzene
(mesitylene)

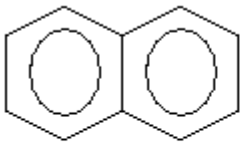


Ethyl benzene

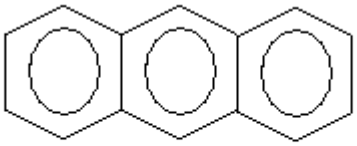


2-propyl benzene

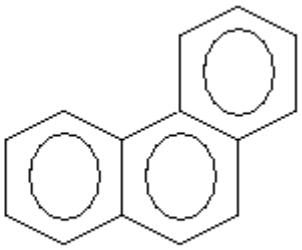
Iso-propyl benzene
or cumene



Naphthalene



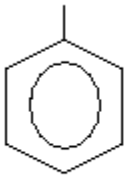
Anthracene



Phenanthere

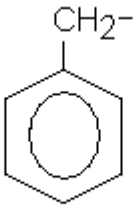
(B) Aryl groups

The radical obtained by removal of one or more hydrogen atoms of the aromatic hydrocarbon molecules are known as aryl group.

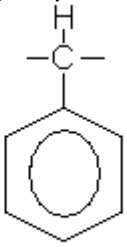


or C_6H_5-

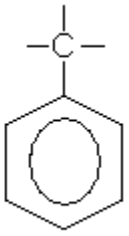
Phenyl



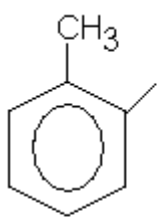
Benzyl



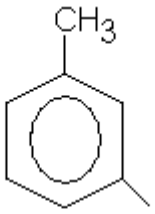
Benzal



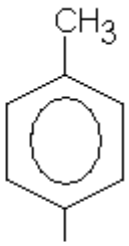
Benzo



O - tolyl or
2 -tolyl



m- tolyl or
3-tolyl

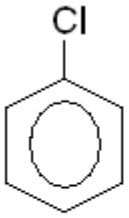


p- tolyl or
4-tolyl

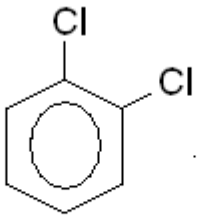
C) Halogen derivatives

(a)Nuclear substitute

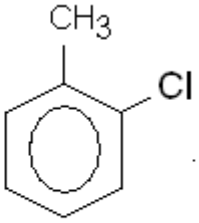
These are the compounds in which substitution on benzene ring with halogen takes place



Chloro benzene



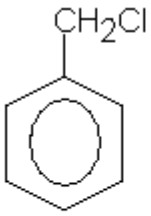
1,2 - Dichlorobenzene
(o-dichlrobenzene)



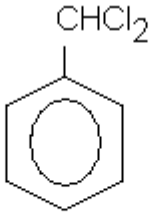
1,2 - Dichlorotoluene
(o-dichrlorotoluene)

(b)Side chain substitute

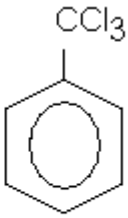
In these compounds, the side chain of the aromatic compound get substituted with halogen e,g.



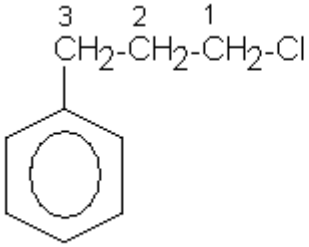
Phenyl chloromethane
(Benzyl chloride)



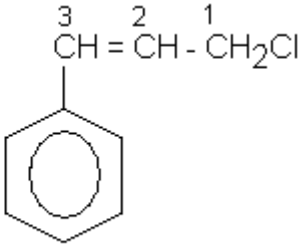
Phenyl dichloromethane
(Benzal dichloride)



Phenyl trichloromethane
(Benzo trichloride)



1-chloro-3-phenyl propane

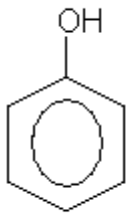


3-chloro-1-phenylprop-1-ene

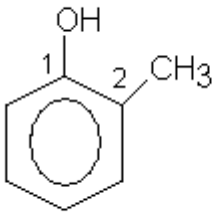
D) Hydroxy derivatives

(a)Nuclear substitute

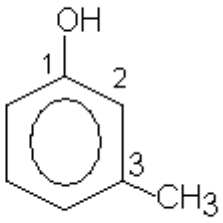
When one or more H-atom of benzene ring get substituted with –OH group we get nuclear substitute aromatic hydroxyl derivative. Which are also known as phenols



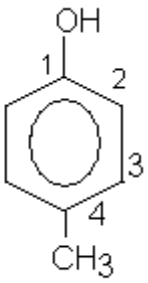
phenol



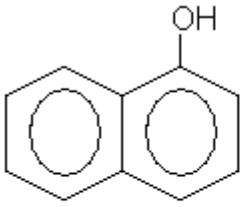
2 - methyl phenol



3 - methyl phenol

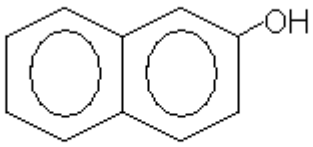


4-methyl phenol



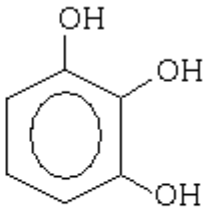
Naphth - 1 -ol

α -Naphthol



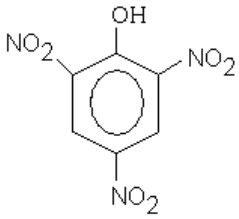
Naphth - 2 -ol

β -Naphthol



Benzene - 1,2,3-triol

Pyrogallol

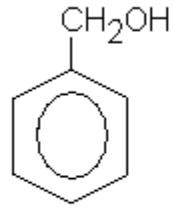


2,4,6 - Trinitrophenol

(Picric acid)

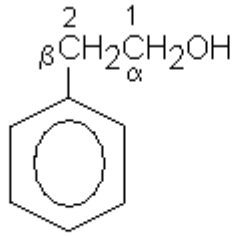
(b) Side chain substituted

In these compounds one or more H-atom of the side chain get substituted with _OH group. These compounds are called aromatic alcohol



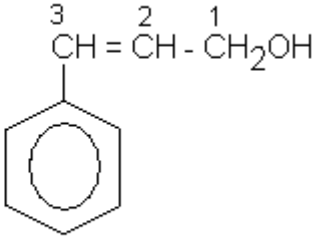
Phenyl methanol

(Benzyl alcohol)



2-Pheyl ethan -1 -ol

β – phenyl ethyl alcohol



3-Phenyl prop-2-en-ol