CHAPTER - 9
ORGANIC CHEMISTRY - NAMING

The word organic signifies life - ie, compounds directly or indirectly derived from living beings.

Berzelius - Vital force theory

Organic compounds are produced only under the influence of some mysterious force existing in living beings.

In 1828 - Wohler discovered urea by heating an inorganic compound.

$$NH_4CNO \xrightarrow[\Delta]{} NH_2 - CO - NH_2$$

Later Kolbe synthesis acetic acid from C and H

Berthelot synthesised methane and acetylene

Thus vital force theory was rejected and it was shown that organic compounds can be synthesised from inorganic source.

Organic chemistry

It is the study about carbon and its compounds or hydrocarbons and their derivatives.

Hydrocarbon classsification

On the basis of nature of carbon skeleton

1. Acyclic or open chain compounds
2. Cyclic or closed chain compounds

I. Acyclic or open chain compounds

Compounds containing open chains of carbon atom in their molecule. It may be straight or branched. These are also known as aliphatic compounds. Further divided into

- Saturated hydrocarbon or alkanes or paraffins

  Compounds containing carbon carbon single bond (C–C)

- Unsaturated hydrocarbon
  - Alkenes or Olefins - Containing C = C
  - Alkynes or Acetylene - Containing C $\equiv$ C

II. Cyclic or closed chain compounds

Compounds containing one or more closed chains or rings of atom

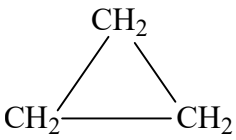
Further divided into

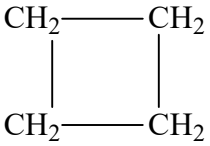
a. Homocyclic :

Rings which are made up of only one kind of atom. Mainly C atom- known as carbocyclic.

i. Alicyclic compounds.

Rings containing 3 or more carbon atom



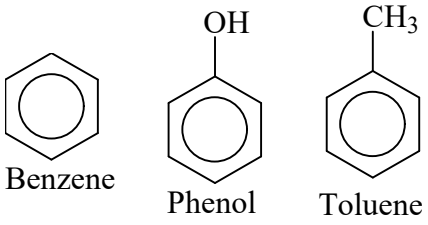


ii. Aromatic compounds.

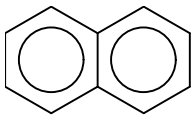
From the greek word Aroma - Fragrant smell

a. Benzenoid aromatic compounds

Aromatic compounds containing one or more fused or isolated benzene rings.

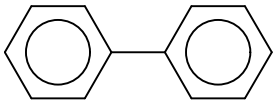


Fused

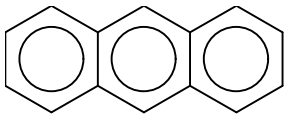


Naphthalene

Isolated



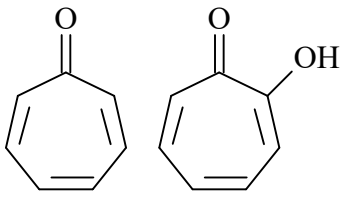
Biphenyl



Anthracene

b. Non-benzenoid aromatic compound

Compounds that does not contain benzene ring but contain other highly unsaturated rings.



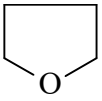
Heterocyclic compounds

Cyclic compounds containing one or more hetero atom in their rings.

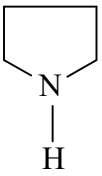
a. Alicyclic heterocyclic

Cyclic compounds containing one or more hetero atom having the properties of corresponding aliphatic compounds

Oxirane



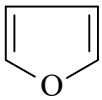
Tetra hydro furan



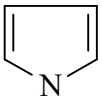
Tetra hydro pyrrole

b. Aromatic heterocyclic

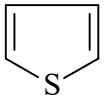
Aromatic cyclic compounds containing one or more hetero atom.



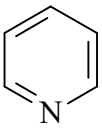
Furan



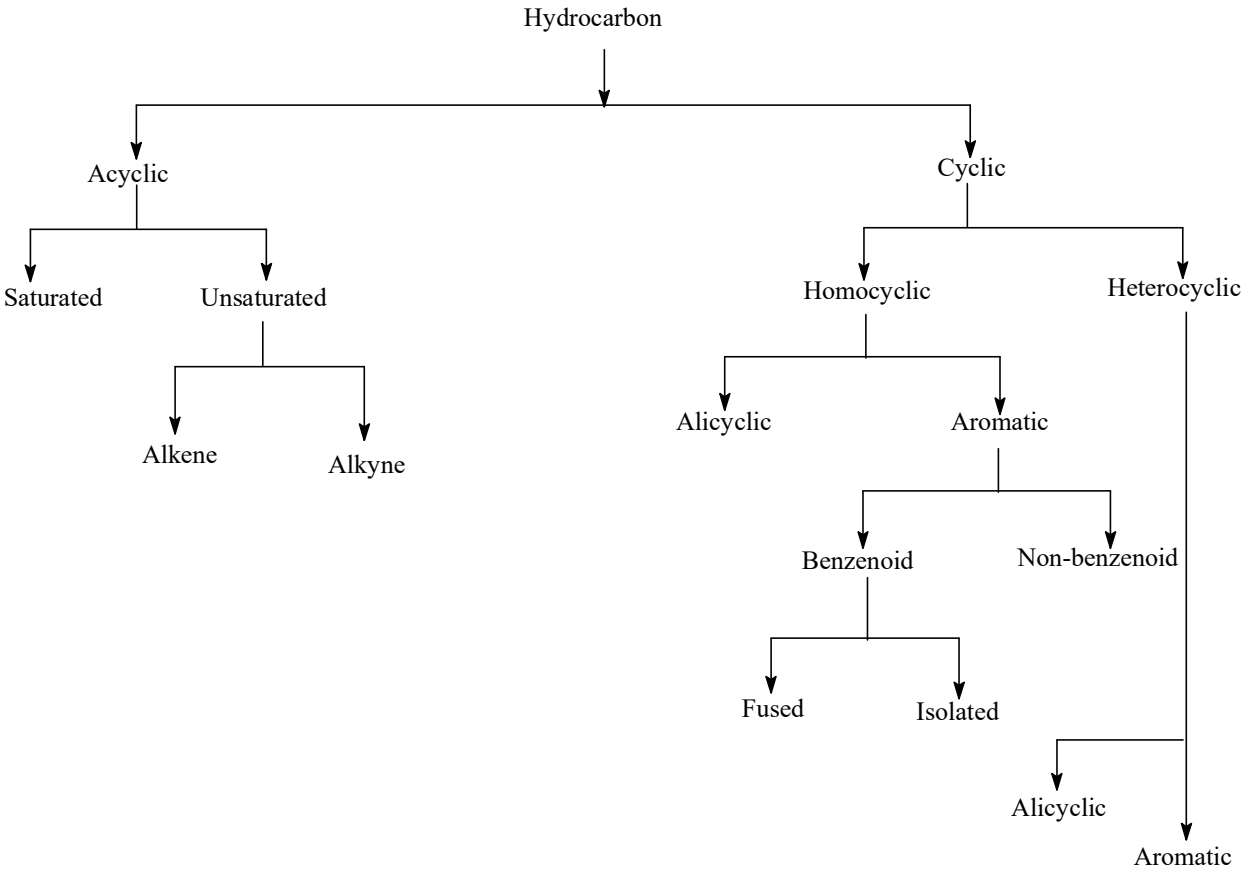
Pyrrole



Thiophene



Pyridine



Nomenclature

System of naming

- Trivial system
- IUPAC system

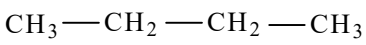
TRIVIAL SYSTEM

Also known as common names.

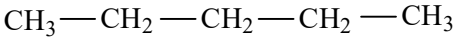
For representing saturated hydrocarbon mainly 3 prefixes are used.

1. n

n - stands for normal or straight chain



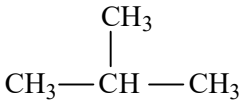
n-butane



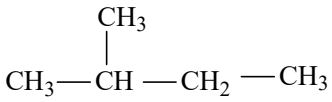
n-pentane

2. Iso

The second carbon containing one methyl group



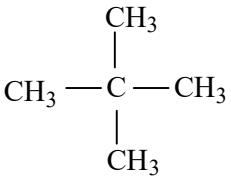
Iso-butane



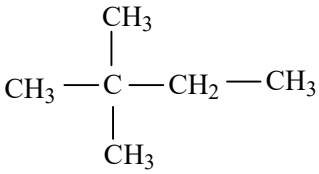
Iso-pentane

3. Neo

Second carbon atom containing 2 methyl group

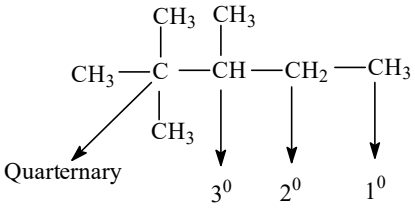


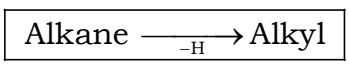
Neo-pentane

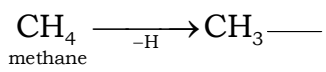


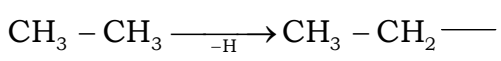
Neo-hexane

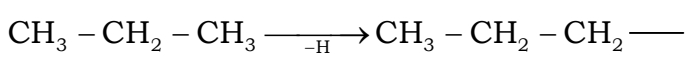
Saturated hydrocarbon contains 4 types of carbon atoms.

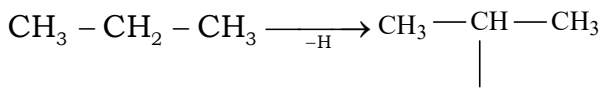


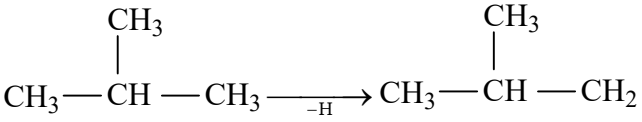


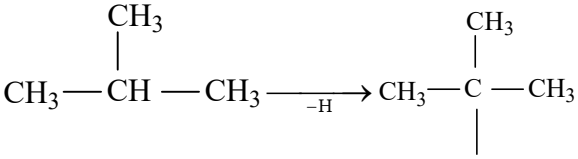

- Methyl


- Ethyl


- Propyl


- Isopropyl


- Isobutyl


- tert-Butyl

IUPAC SYSTEM

In 1892 an International Chemical Congress was held at Geneva, they started a new naming system for organic compounds known as Geneva system of Nomenclature. This system was further modified as IUPAC nomenclature.

Rules

Each systematic name contain

- Word root; • Suffix; • Prefix

Word root :

It denote no.of carbon atoms in the parent chain.

Primary suffix

It shows saturation or unsaturation in a chain

Nature of C-chain	**1° suffix**
C–C	–ane
C=C	–ene
C≡C	–yne

Secondary suffix

It indicates the presence of a particular group (functional group)

Functional group	2° suffix
Alcohol	–ol
Aldehyde	–al
Ketone	–one

Primary prefix

It is used to distinguish cyclic from acyclic compound. In case of carbocyclic compound, 1° prefix cyclo is used.

Secondary prefix

It denote the presence of substitutent or side chain on the parent chain.

–X	halo
$-NO_2$	Nitro
–R	Alkyl
–OR	Alkoxy

The complete IUPAC name of compound contain:

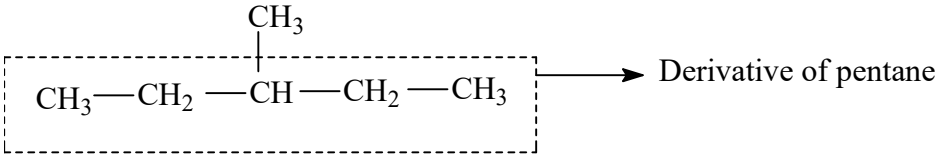
2° prefix + 1° prefix + word root + 1° suffix + 2° suffix

Eg : 2-methyl butanoic acid $\Rightarrow$ Methyl $\rightarrow$ 2° prefix : but - word root : an $\rightarrow$ 1° suffix : oic acid-2° suffix

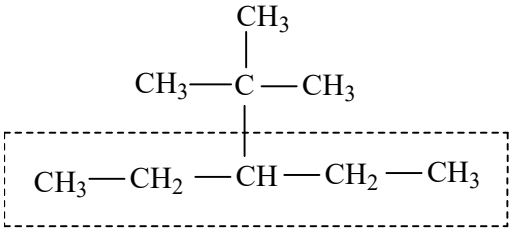
NAMING OF COMPLEX COMPOUNDS

- **Longest chain rule**

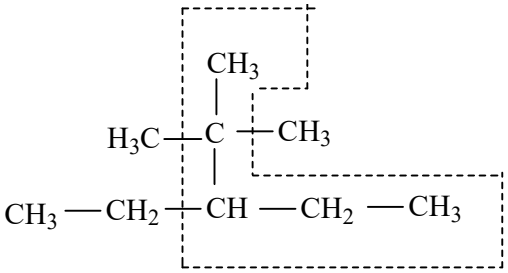
Select the longest continuous chain of carbon atom in the molecule. The continuous chain of carbon atom is called parent chain or main chain. Carbon atom which are not included in the parent chain are considered as substituent or side chain.



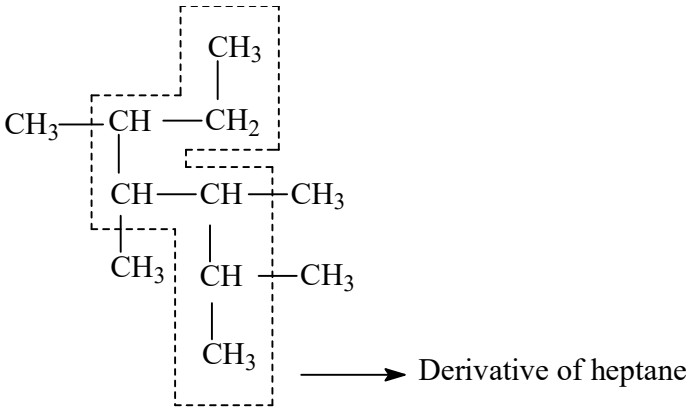
- Two or more carbon chains of equal length, then the selected chain should contain maximum no.of side chain or substituent.



1- side chain



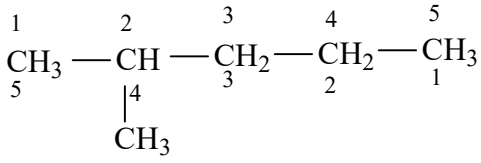
3- side chain (correct way)



- **Numbering of carbon chain**

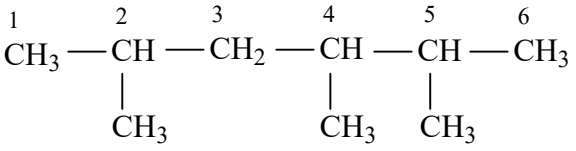
The carbon atoms of longest continuous chains are numbered. The no that indicate the position of substituent is known as Locants.

The carbon atom carrying first substituent get the lowest possible locants.

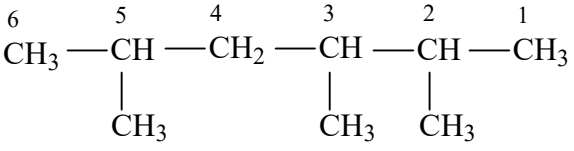


2-Methylpentane (correct); 4-methyl pentane (wrong)

Two or more substituents are attached to the parent chain, lowest set of locant is preferred. The lowest set is determined by **first point of difference rule.** The rule says "when two or more different set of locants containing same no.of term is possible, then the set of locants is compared term by term with other set, each set in order of increasing magnitude. The set of locant is preferred which has a lower no.at the first point of difference".



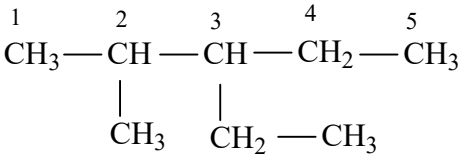
(2, 4, 5)



(2, 3, 5) lowest set

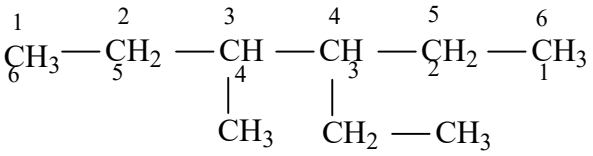
2,3,5-Trimethyl hexane

- If there are different alkyl substituents attached to the parent chain, their names are written in alphabetical order.



- 3-Ethyl-2-methyl pentane

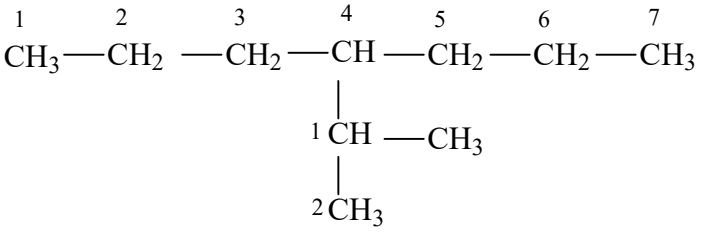
- If there are different alkyl substituent at equivalent positions the numbering is done in such a way that the substituent which comes first in alphabetical order get lowest possible number.



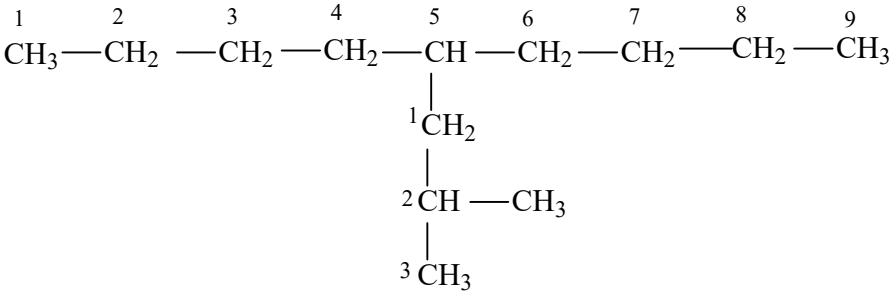
3-Ethyl-4-methylhexane

Naming of complex alkyl substituents

If the substituent on the parent chain is a complex, the carbon atom of this group attached to the parent chain is given as 1.

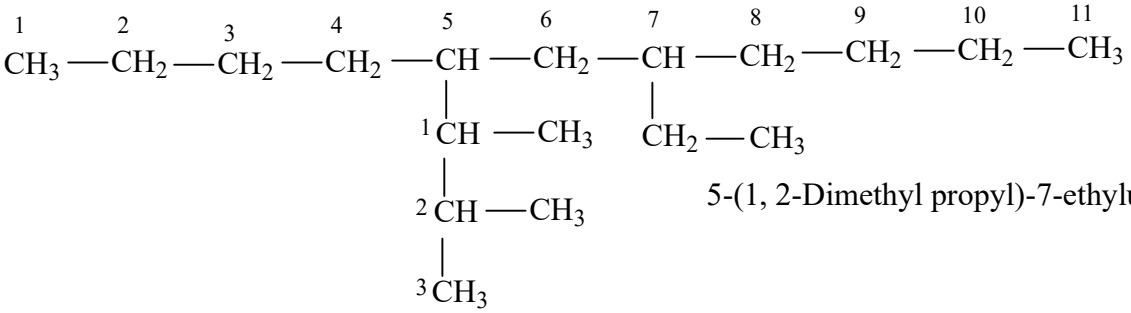


4- (1-methyl ethyl)heptane
or
4-isopropyl heptane

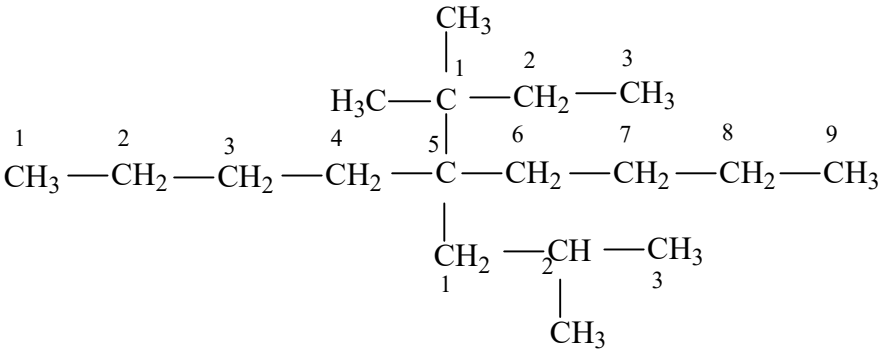


5- (2-methylpropyl)nonane
or
5-isobutyl nonane

- While deciding the alphabetical order of various substituents, the name of complex substituent is considered to begin with first letter of complex name.

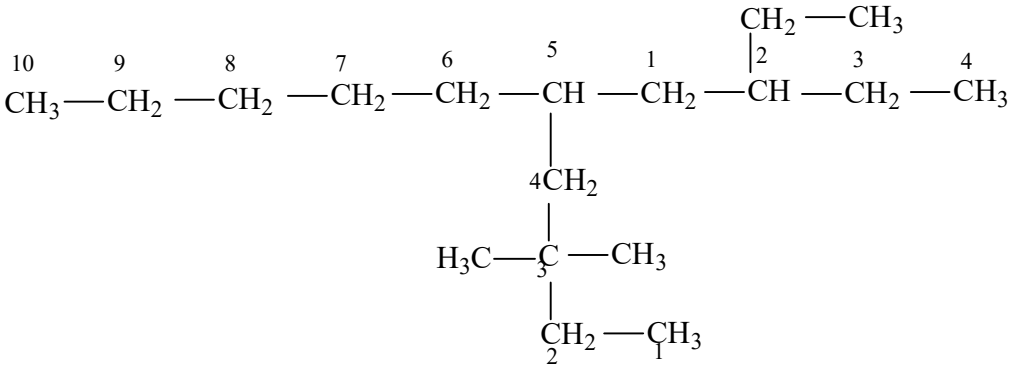


5-(1, 2-Dimethyl propyl)-7-ethylundecane



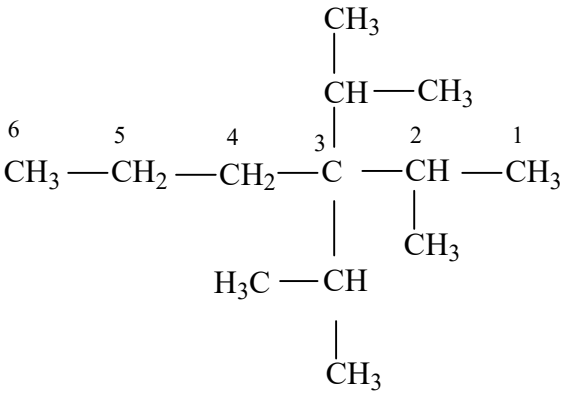
5-(1, 1-Dimethyl propyl)-5- (2-methylpropyl)nonane

- If two complex substituents are of equal length, then the complex substituent with larger no.of alkyl group form a part of longest carbon chain while the other one considered as complex substituents.



5-(2-Ethylbutyl)-3,3-dimethyldecane

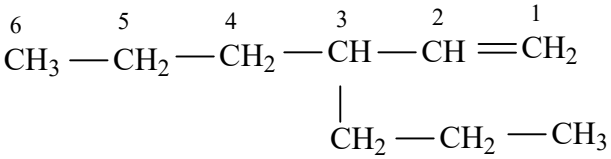
- If same complex substituent occur more than once prefix such as bis(2), tris(3), tetra kis (4)..... etc are used before the name of complex name.



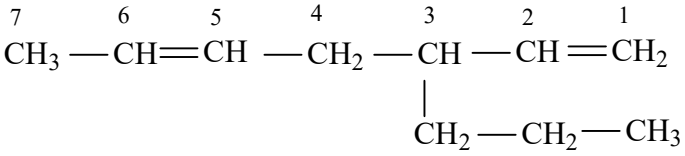
2-methyl-3,3-bis(1-methylethyl) hexane

Naming of unsaturated compound

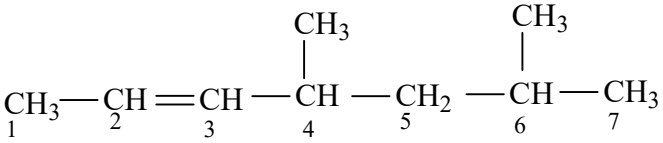
- Longest chain of carbon atom is selected to included the double or triple bond, even if it is not the actual longest chain



- If more than one double or triple bond is present in the molecule, the selected chain should contain maximum number of such bonds.

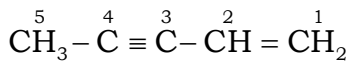


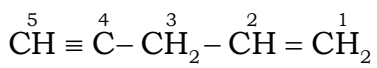
- The parent chain is numbered in a manner to give lowest number to that carbon atom linked by a double or triple bond.

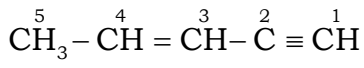


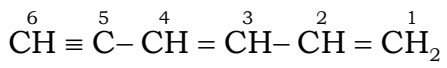
4,6-Dimethyl hept-2-ene

- If a compound contains both double and triple bond, such compounds are named as **Alkenynes.**

 Pent-1-en-3-yne

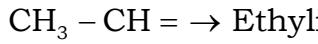
 Pent-1-en-4-yne

 Pent-3-en-1-yne

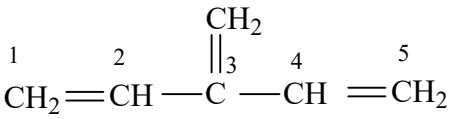
 Hexa-1,3-dien-5-yne

In some cases all the double and triple bond are not included in the parent chain, in such cases,.....

are used

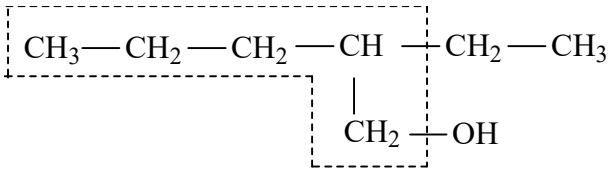


3-Methylene penta-1,4-diene

Naming of compounds containing one functional group.

- **Longest chain**

  The selected parent chain should be the one containing functional group.



- **Numbering of carbon chain**

  The carbon linking to functional group get the lowest possible number.

  When a chain terminating group such as –CHO, –COOH, –COOR, –$CONH_2$, –CN are present as functional group it must be assigned as number 1.

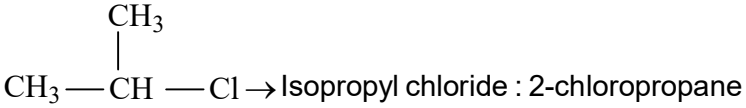
- Numerical prefix like di, tri, tetra etc are attached before the suffix name if the same functional group occur more than once.

Alkyl halide

R – X **CN :** Alkyl halide

IUPAC : Haloalkane

$CH_3 - CH_2 - Br \rightarrow$ Ethylbromide; Bromoethane



Alcohol

R–OH CN : Alkylalcohol

IUPAC : Alkanol

CH_3-OH $\rightarrow$ Methanol; Methylalcohol

CH_3-CH_2-CH_2-OH $\rightarrow$ Propanol; Propylalcohol

Ether

R–O–R CN : Dialkylether

IUPAC : Alkoxy alkane

$CH_3 - O - CH_3 \rightarrow$ Dimethyl ether
Methoxy methane

$CH_3 - O - C_2H_5 \rightarrow$ Ethyl methyl ether
$\rightarrow$ Methoxy ethane

Carboxylic acid

–COOH

CN : Obtained from the source from which they were isolated or present in large quantity.

IUPAC : Alkanoic acid

$H - COOH \rightarrow$ Formic acid
Methanoic acid

$CH_3COOH \rightarrow$ Acetic acid
Ethanoic acid

$CH_3CH_2COOH \rightarrow$ Propionic acid
Propanoic acid

$CH_3CH_2CH_2COOH \rightarrow$ Butyric acid
Butanoic acid

Aldehyde

- CHO

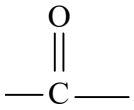
CN : Replace the terminal -ic acid in corresponding acid by aldehyde

IUPAC : Alkanal

H – CHO $\rightarrow$ Formaldehyde ; Methanal

$CH_3CHO \rightarrow$ Acetaldehyde ; Ethanal

Ketone



CN : Dialkylketone

IUPAC : Alkanone

$CH_3 - CO - CH_3 \rightarrow$ Dimethyl ketone (Acetone) ; Propanone

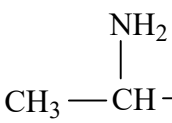
Amine

$-NH_2$

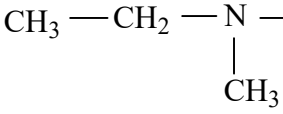
CN : Alkylamine

IUPAC : Alkanamine

$CH_3\text{-}NH_2 \rightarrow$ Methyl amine
Methanamine

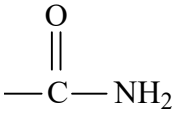

: Isopropylamine
Propan-2-amine

$CH_3 - NH - CH_3 \rightarrow$ N – methylmethanamine



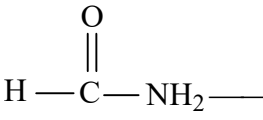
→ N,N-Dimethylethanamine

Amide

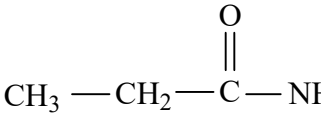


CN : replace -ic acid by amide

IUPAC : Alkanamide

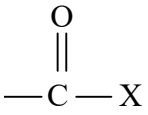


⟶ Formamide : Methanamide



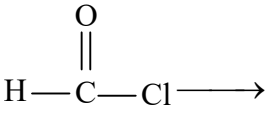
⟶ N-Methylpropanamide

Acid halide

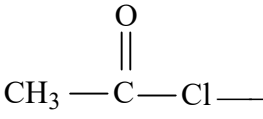


CN : Replace -ic acid by -yl halide

IUPAC : Alkanoyl halide

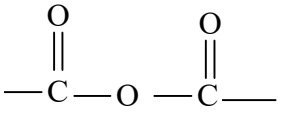


⟶ Formyl chloride : Methanoyl chloride

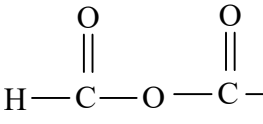


⟶ Acetyl chloride : Ethanoylchloride

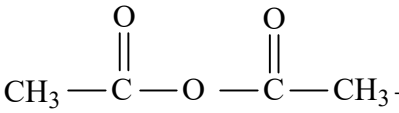
Acid anhydride



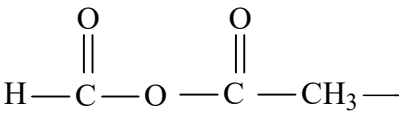
CN : Replace acid by anhydride; IUPAC : Alkanoic anhydride



⟶ Formic anhydride : Methanoic anhydride

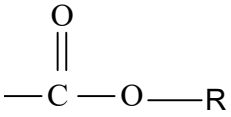


⟶ Acetic anhydride : Ethanoic anhydride



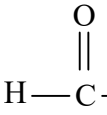
⟶ Acetic formic anhydride : Ethanoic methanoic anhydride

Ester

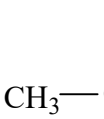


CN : Replace - ic acid by ate

IUPAC : Alkyl alkanoate



: Methyl formate : Methylmethanoate



: Methylacetate : Methylethanoate

Naming of compounds containing more than one functional group

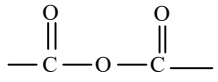
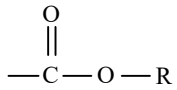
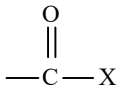
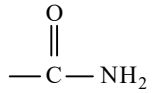
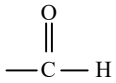
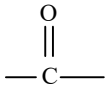
A compound containing more than one functional group or more than one multiple bond is considered as poly functional compounds.

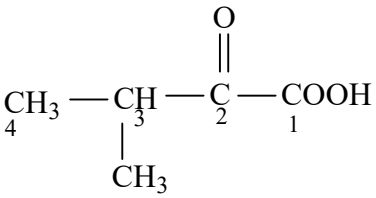
In such compounds one functional group is considered as principal functional group and others are substituents. The principle functional group is mentioned by its suffix name and substituent is mentioned by its prefix name

Rules

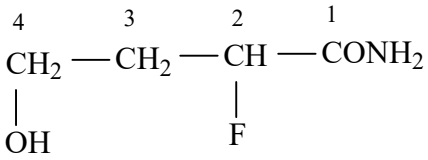
- Select the principal functional group
- Select the parent chain, it include principal functional group (PFG)
- Numbering the chain, PFG get lowest possible number.

Numbering preference order $\text{PFG} > = > \equiv > \text{substituent}$

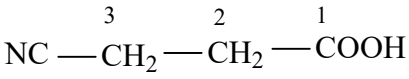
Functional group	Prefix name	Suffix name
$-COOH$	Carboxy	-oic acid
$-SO_3H$	Sulpho	Sulphonic acid
	-	-oic anhydride
	Alkoxy carbonyl	-oate
	Halocarbonyl	-oyl halide
	Carbamoyl	-amide
$-CN$	Cyano	-nitrile
	Formyl/oxo	-al
	Keto/oxo	-one
$-OH$	Hydroxy	-ol
$-SH$	Mercapto	thiol
$-NH_2$	Amino	-amine
$-C=C-$	-	alkene
$-C\equiv C-$	-	alkyne
$-R$	Alkyl	-
$-OR$	Alkoxy	-
$-NO_2$	Nitro	-
$-NO$	Nitroso	-
$-N=N-$	Diazo	-
$-X$	halo	-



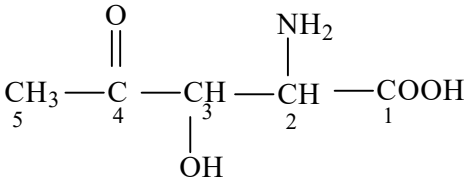
3-Methyl-2-oxobutanoic acid



2-Fluoro-4-hydroxy butanamide



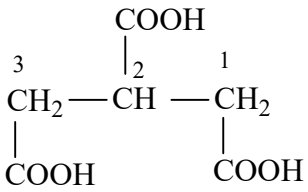
3-Cyano propanoic acid



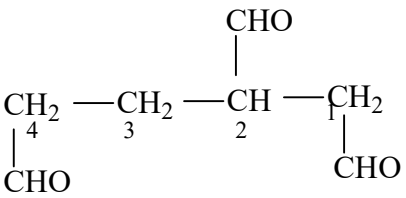
2-Amino-3-hydroxy-4-oxopentanoic acid

Poly functional compounds containing more than two like functional group

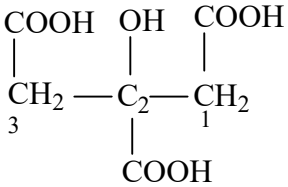
If an unbranched carbon chain is directly linked to more than two like functional group, the compound is named as the derivative of parent alkane, the carbon atoms of like functional group do not include in the numbering, in such case suffix like carboxylic acid (COOH), carbaldehyde (CHO), carbonitrile (CN) etc are used.



Propane-1,2,3-tricarboxylic acid

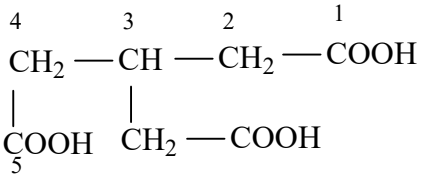


Butane-1,2,4-tricarbaldehyde

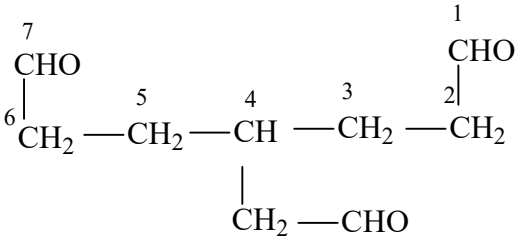


2-Hydroxy propane-1,2,3-tricarboxylic acid

If more than 2 like functional group is not directly linked to the carbon chain, then the carbon atoms of functional group directly attached to the parent chain is included in numbering, the other one is considered as substituent group.



3-(carboxymethyl)-pentane-1,5-dioic acid

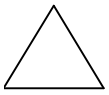


4-(Formylmethyl)heptane-1,7-dial
4-(2-oxoethyl)heptane-1,7-dial

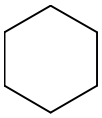
Naming of alicyclic compound

- **Cycloalkane**

Names obtained by adding the prefix 'cyclo' before the name of a corresponding alkane.



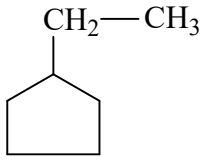
Cyclopropane



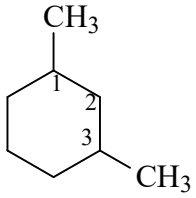
Cyclohexane

Alkyl substituted cycloalkane are known as "**alkylcycloalkane**".

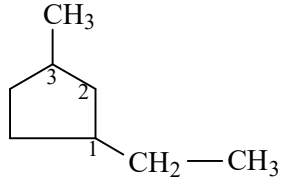
If different substituents are present their names are written in alphabetical order. Numbering is done in such a way that substituent which comes first in alphabetical order get lowest possible number. Numbering does not violate lowest set of locant rule.



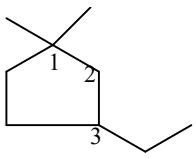
Ethylcyclopentane



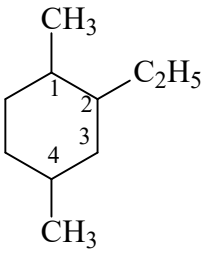
1,3-Dimethyl cyclohexane



1-Ethyl-3-methyl cyclopentane

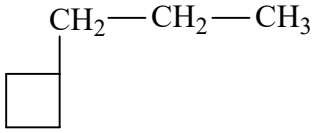


3-Ethyl-1,1-dimethyl cyclopentane

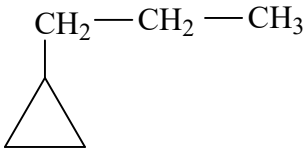


2-Ethyl-1,4-dimethyl cyclohexane

The ring containing more or equal number of carbon atom than alkyl group, then the compound is named as derivatives of ring.

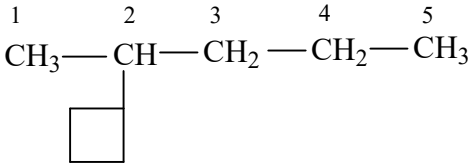


Propyl cyclobutane

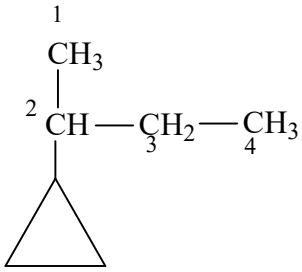


Propyl cyclopropane

If the side chain contains more no.of carbon atom than the ring, compound is derivative of side chain.

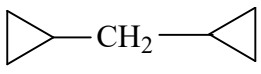


2-Cyclobutyl pentane

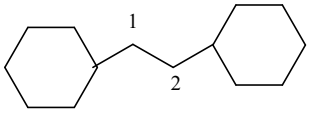


2-Cyclopropyl butane

If more than one alicyclic ring is directly attached to the carbon chain, compound is derivative of carbon chain.



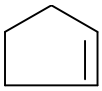
Dicyclopropylmethane



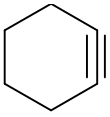
1,2-Dicyclohexyl ethane

Cycloalkene and cycloalkyne

Adding the prefix cyclo before the name of the corresponding alkene or alkyne.

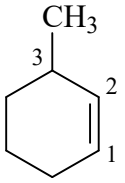


Cyclopentene

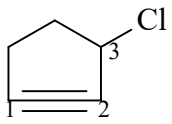


Cyclohexyne

In case of substituted cycloalkene and cycloalkyne the number of double and triple bond get lowest possible number 1 and 2 and the substituent get lowest possible no at first point of difference rule.



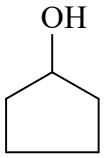
3-Methylcyclohexene



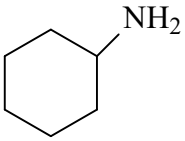
3-Chlorocyclopentyne

Alicyclic compounds containing functional group

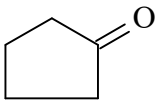
Alicyclic alcohol, amines, ketones ..... are named as corresponding aliphatic compounds by prefixing the word cyclo.



Cyclopentanol



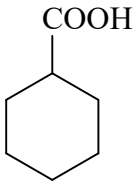
Cyclohexanamine



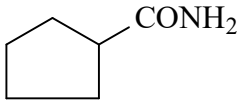
Cyclopentanone

If an alicyclic ring is directly attached to a carbon containing functional group, the carbon atom of the functional group is not included in the parent chain. In such cases following suffix and prefix are used

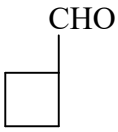
Functional group	**Prefix**	**Suffix**
–COOH	Carboxy	Carboxylic acid
–CHO	Formyl	Carbaldehyde
–COX	Halocarbonyl	Carbonylhalide
–CN	Cyano	Carbonitrile
$–CONH_2$	Carbamoyl	Carboxamide
–COOR	Alkoxy carbonyl	carboxylate



Cyclohexane carboxylic acid

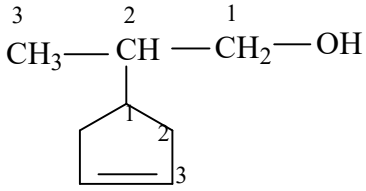


Cyclopentane carboxamide



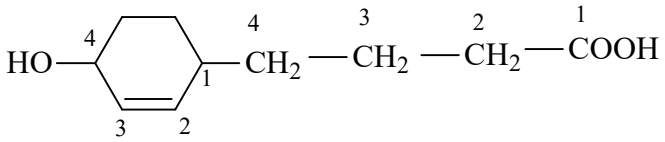
Cyclobutane carbaldehyde

If a ring containing a multiple bond and the side chain containing functional group, then the compound is derivative of side chain.



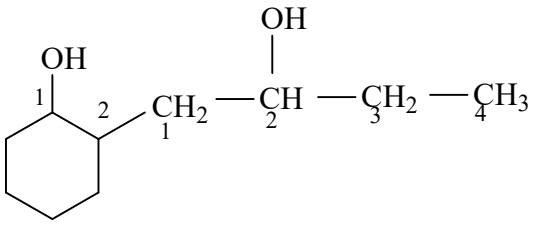
2-(Cyclopent-3-enyl) propanol

If the ring and side chain contains functional group then the compound is named as derivatives of ring or side chain which will contain principal functional group.

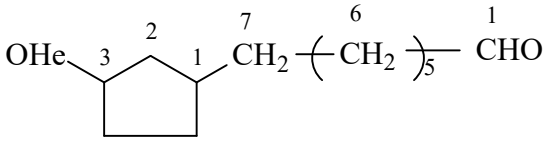


4-(4-Hydroxycyclohex-2-enyl)butanoic acid

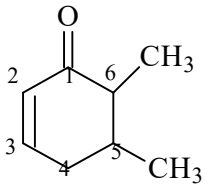
If the ring and side chain contains same functional group, the compound is named as a derivative of side chain or the ring, which containmore number of carbon atom.



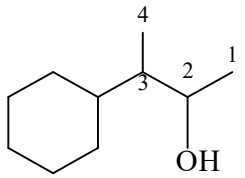
2-(2-Hydroxybutyl)cyclohexanol



7-(3-Formylcyclopentyl)heptanal



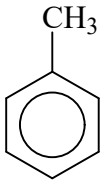
5,6— Dimethyl cyclo hex–2 – en – 1 – one



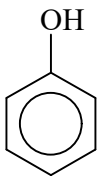
3 — Cyclohexylbutan–2 – ol

Nomenclature of Aromatic compound

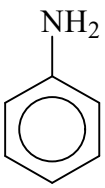
Compounds are derivatives of **benzene**. The names are obtained by “substituent name + benzene”. Most of the compounds have typical names.



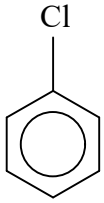
Methylbenzene (Toluene)



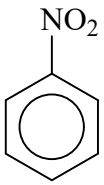
(Phenol)



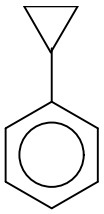
(Aniline)



Chlorobenzene

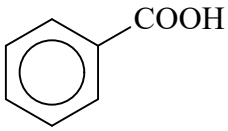


Nitrobenzene

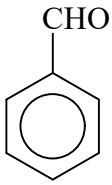


Cyclopropyl benzene

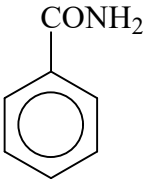
Special case



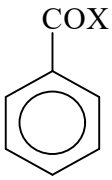
Benzene carboxylic acid
(Benzoic acid)



Benzene carbaldehyde
(Benzaldehyde)

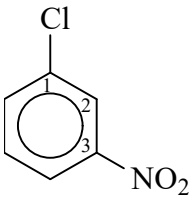


Benzene carboxamide
(Benzamide)

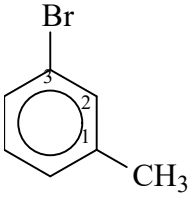


Benzene carbonylhalide
(Benzoylhalide)

- If more than one substituents are present names are written in alphabetical order
- If any of the substituent give a special name to the compound, then compound is derivative of that special name.
- Numbering does not violate lowest set of locant rule.

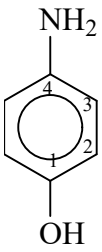


1-Chloro-3-nitrobenzene

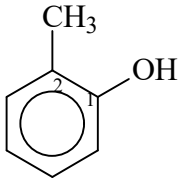


3-bromo toluene, (m-bromotoluene)

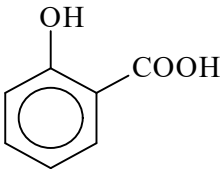
(The position number is indicated in IUPAC system but position name is indicated in common system)



4-Amino phenol
p-Amino phenol

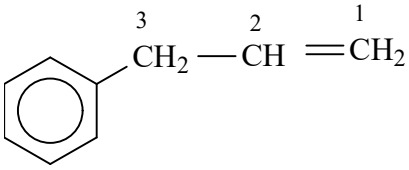


2-Methyl phenol
o-methyl phenol(O-cresol)

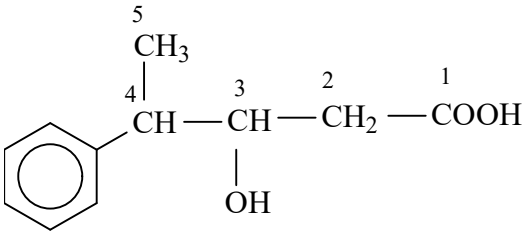


2-Hydroxybenzoic acid
o-hydroxy benzoic acid (salicylic acid)

If benzene ring is attached to an aliphatic chain containing a multiple bond or functional group or substituent, benzene ring is considered as a substituent group known by phenyl.



3-Phenyl prop-1-ene



3-Hydroxy-4-phenylpentanoic acid