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General Organic Chemistry & Isomerism

Vital force theory :

Organic compounds can be made only from natural sources. It was given by Berzelius.

Wholer synthesis :

He made urea, the first organic compound made in Labouratory from inorganic sources.

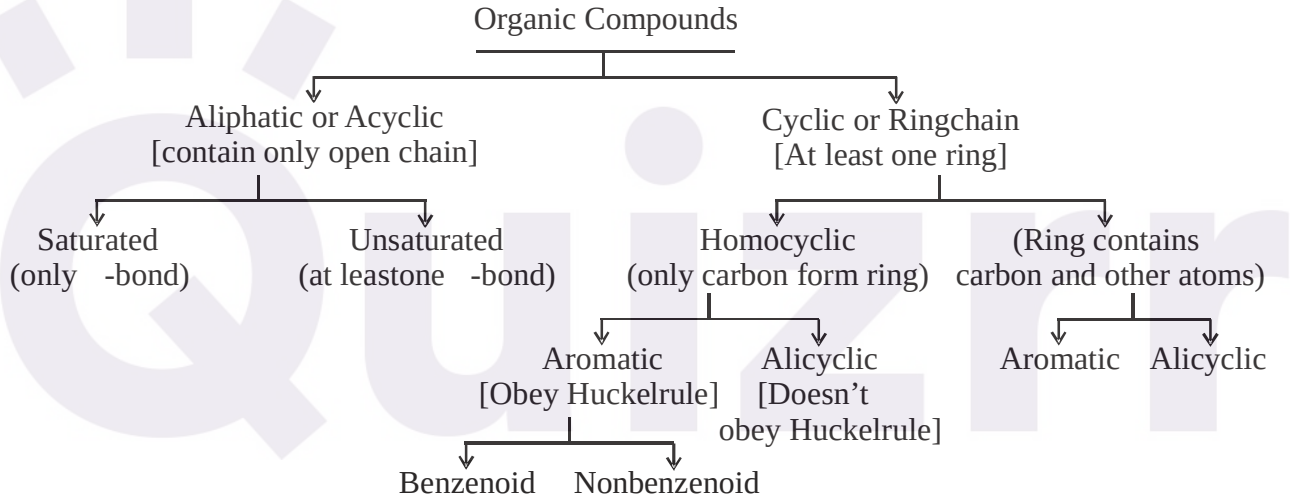
$$NH_4Cl + KCNO \longrightarrow KCl + NH_4CNO$$

$$\downarrow \text{rearrange}$$

$$H_2N\text{–}\underset{\displaystyle O}{\overset{\displaystyle \|}{C}}\text{–}NH_2$$

(Urea)

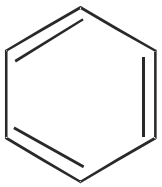
Organic Compound : Hydrocarbon and their derivatives are called as organic compounds.



Nonmenclautre : → Trivial system; → IUPAC system

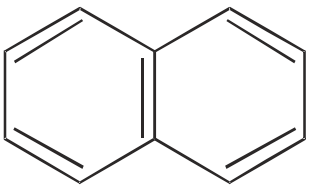
Aromatic Compounds :

Earliear, compounds with pleasant smell were called Aromatic compounds. Now a days the termaromatic means planar cyclic molecule or ion containing delocalised π-electrons, must follow Huckel's rule ie $(4n+2)\pi$ electrons, resist addition reaction, gives electrophilic substitution reaction. In Huckel's rule n = any whole number ie 0, 1, 2, ...



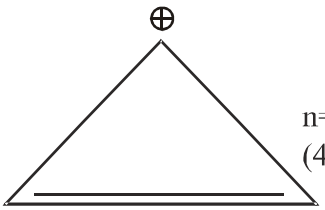
n=1
$4n+2 = 6\pi$electrons

Benzene

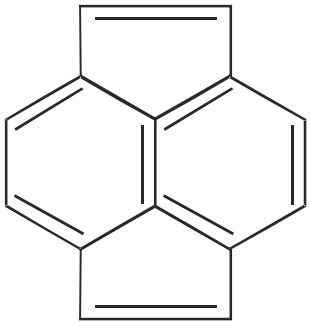


n=2
4n + 2 = 10p electrons

Naphthalene



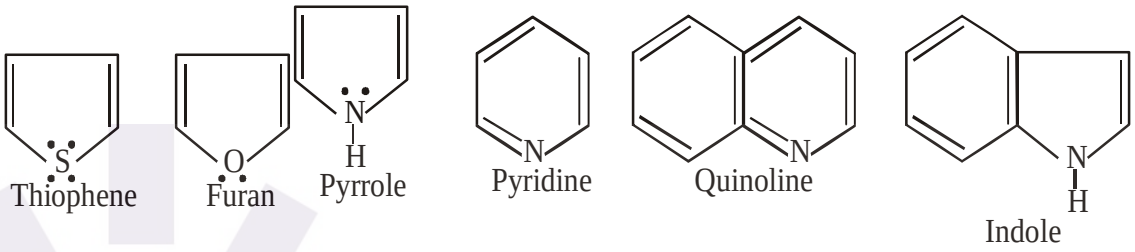
n=0
(4n+2) = 2πelectrons



n=3
4n+2 = 14 πelectrons

Aromatic Heterocyclic Compounds :

Atomatic compounds which contain a hetero atom (O, S, N etc.) in the ring are called heterocyclic compound e.g.

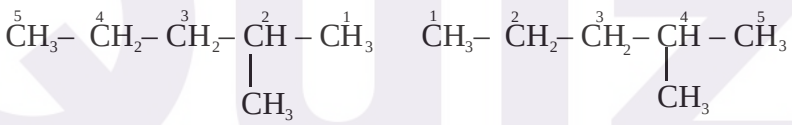


A. Numbering of the carbon atoms of the longest chain :

(a) Lowest individiual number or lowest locant rule :

The carbon atoms carrying the first substituent get the lowest possible number.

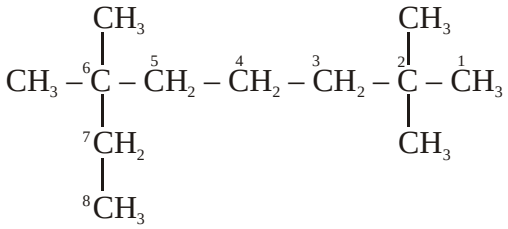
e.g.



2-Methylpentane (Correct) 4-Methylpentane (wrong)

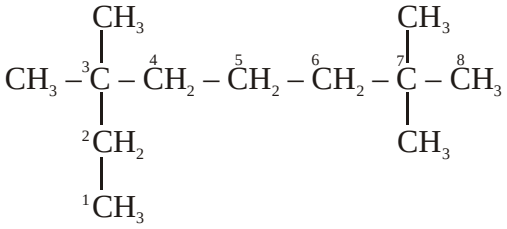
(b) Lowest Sum Rule :

When many substituents are present, the numbering is done from the end where upon the sum of locants is the lowest.



2, 2, 6, 6-Tetramethyloctane (correct)

Sum of locants = 2 + 2 + 6 + 6 = 16

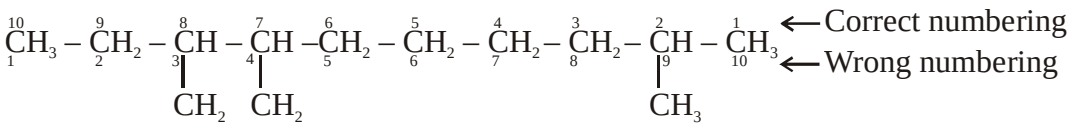


3,3,7,7-Tetramethyloctane (wrong)

Sum of locants = 3 + 3 + 7 + 7 = 20

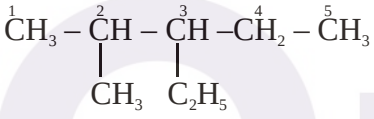
(c) First point of difference rule :

For a very long carbon chain, the set of locant is preferred which has a lower number at the first point of difference even, if it violates the lowest sum rule.

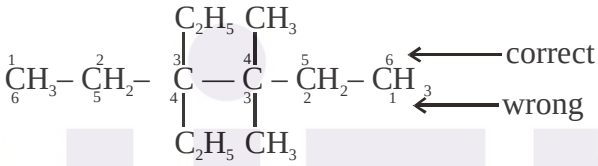


(d) Alphabetical order of simple substituents :

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



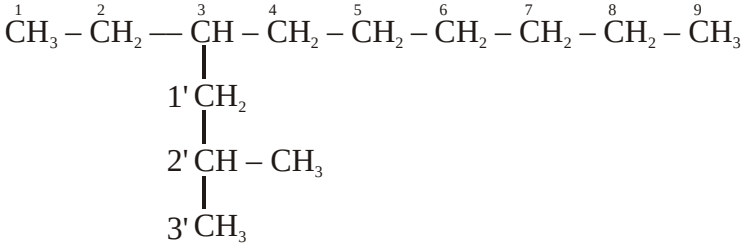
3-Ethyl-2-methylpentane



3,3-Diethyl-4, 4-dimethylhexane

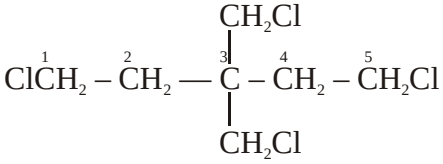
B. Naming the Complex Alkyl Substituents

When the substituents on the parent chain is itself branched chain, it is named as substituted alkyl group and its carbon chain is separately numbered in such a way, that the carbon atom directly attached to the parent chain is given number 1'. The name of this complex substituents is written in brackets.



3–(2'methylpropyl)nonane

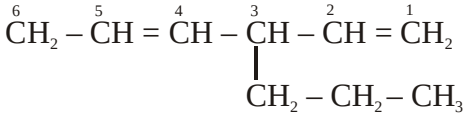
Note : The numerical prefixes ‘bis’, ‘tris’, ‘tetrakis etc. are used to indicate a multiplicity of substituted substituent.



3,3–Bis (Chloromethyl)-1,5-dichloropentane

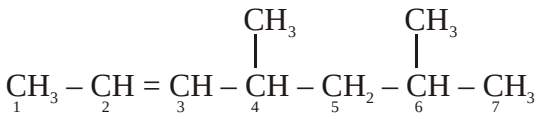
C. Rules ;for having complex unsaturated Aliphatic Hydrocarbons

(i) Longest chain : The longest chain of carbon atoms (parent chain) is so selected as to include the double or triple bond even if it is not the actual longest chain of carbon atoms.



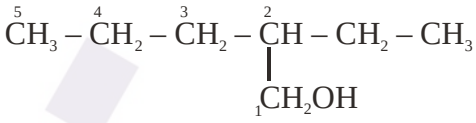
3 – Propylhexa - 1,4-diene

(ii) Numbering of carbon chain : The parent carbon chain is numbered in such a manner so as to give lowest number to that carbon atom linked by double or triple bond even if it violates the rules of saturated hydrocarbons.



4,6-Dimethylhept-2-ene

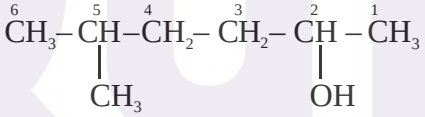
D. Rules for Naming Complex Aliphatic Compounds Containing one Functional Group :



2-Ethylpentam-1-o1

Numbering of Parent Chain

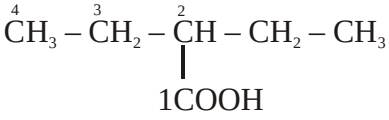
The numbering of the parent carbon chain is done in such a way that the carbon linking to functional group gets the lowest number even if there is violation of saturated hydrocarbon rules.



5,5 - Dimethlhexan-2-ol

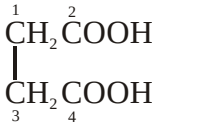
Note:

(i) When a chain terminating group such as –CHO, –COOH, –COOR, $–CONH_2$, $–C\equiv N$, etc is present as the functional group, it must be assigned number 1. This does not apply to non-terminal groups such as >CO, $–NH_2$ and –OH from first position may or may not be assigned.

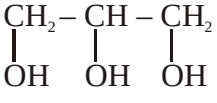


2-Ethylbutanoic acid

(ii) Numerical prefixes di-, tri-, tetra etc are attached before the designations of functional group if two or more identical groups are present. e.g.

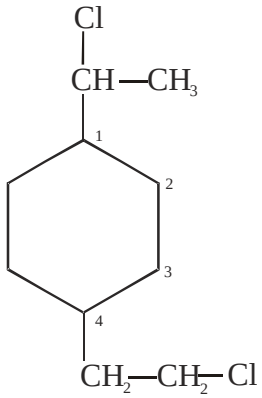


Butane-1,4-dioic acid



Propane – 1,2,3 - triol

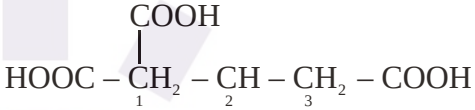
(iii) When two or more prefixes consists of identical roman letters, priority is given to the group which contains the lowest locant at the first point difference. e.g.



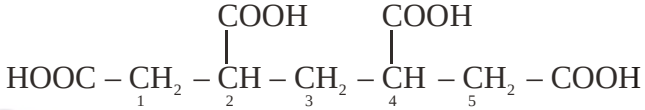
1-(1'-chloroethyl)-4-(2'-chloroethyl) cyclohexane

Here 1'-chloroethyl gets priority over 2'-chloroethyl.

(iv) If unbranched chain is linked directly to more than two carboxyl groups, these groups are named by substitutive use of suffix "tricarboxylic acid" etc. The principal chain selected should be linked directly to maximum possible number of carboxyl groups e.g.

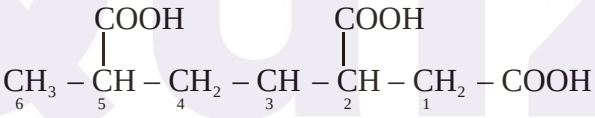


Butane 1, 2, 3-tricarboxylic acid



Pentane–1,2,4,5–tetracarboxylic acid

(v) The carboxylic groups which are not directly linked to the principal chain are expressed as carboxyalkyl prefixes e.g.



3-(carboxymethyl)hexane-1,2,5-tricarboyxlic acid

Similarly, the substitutive prefixes for aldehyde, cyanides, acylchlorides and amides are carbaldehyde carbonitrile, chlorocarbonyl and carboxamide respectively.

E. Rules for Naming Aliphatic Compounds Having Polyfunctional Groups

A compound containing more than one functional group is called polyfunctional compound. In IUPAC system, one of the functional groups is chosen as the principal function group (secondary suffix) and the remaining functional groups (secondary functional groups) are treated as substituents and indicated by prefixes.

The choice of the principal functional group is made on the basis of the following order of preference.

Carboxylic acid > sulphonic acid > acid anhydrides > esters > acid chlorides > acid amides > cyanides > aldehydes . ketones > alcohols, phenols, thiols > amines > alkenes > alkynes > halo, nitro, alkyl

Seniority Table for Principal groups

(Highest priority group at the top)

Group	Prefix Name	Suffix Name
–COOH	Carboxy	-oic acid
$–SO_3H$	Sulpho	Sulphonic acid

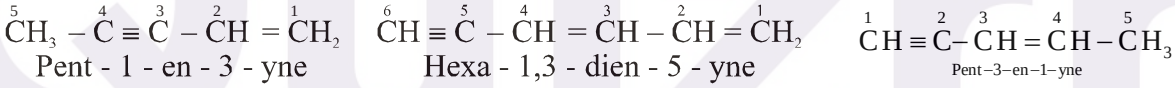
–COOR	Alkoxy carbonyl or Carbalkoxy	oate
–COX	Haloformyl or Halocarbonyl	-oyl halide
$-CONH_2$	Carbamoyl	amide
–CN	Cyano	nitrile
–NC	Isocyano	Carbylamine
–CHO	Formyl or aldo	-al
>C = O	Keto or oxo	-one
–OH	Hydroxy	-ol
–SH	Mercapto	Thiol
$-NH_2$	Amino	amine
>C = C<	-	-ene
$-C \equiv C-$	-	yne

1. The first step in the naming of polyfunctional compounds is the selection of principal functional group which gives the class name of the structure.
2. The second step is the selection of parent chain as such it includes the maximum number of functional group including the principal group.
3. The third step is the numbering of parent chain. Which is done from the side of principal functional group i.e. it gets lowest number. The following decreasing order of preference for giving thelowest numbers is followed.

   Principal functional group > Double bond or Triple bond > Substituents.

Note :

(a) If a molecule contains both carbon-carbon double and triple bonds, preference of numbering is generally given from the double bond side. But in one case when triple bond is present at the terminal position and double bond at any where in central position, then numbering should be done from triple bond side.



Pent - 1 - en - 3 - yne Hexa - 1,3 - dien - 5 - yne Pent–3–en–1–yne

(b) In case two substitutents of same seniority occupy identical position in relation to the end of the chain, the lower number should be given to the substituent in alphabetical order.

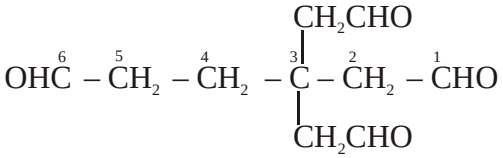
$ClCH_2CH_2CH_2Br$

1-Bromo-3-Chloropropane

4. If all the like groups are not directly linked to the unbranched carbon chain, the carbon atoms of the two like groups are included in the present chain while the third which forms the side chain is considered substitutent group.

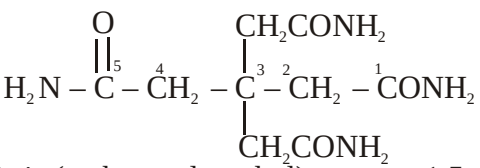
   e.g.

(i)



3,3-Bis (formylmethyl) hexane-1, 6-dial

(ii)



3,3-Bis is (carbamoyl methyl) pentane-1,5-diamide

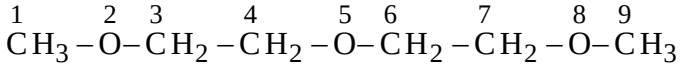
F. Replacement Nomenclature

In this system, ethers, sulphides, selenides and amines are named as oxa, thia, selena and aza derivatives of alkane corresponding to the total number of carbon and oxygen or sulphur or selenium or nitrogen atoms.

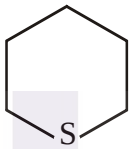
The location of these hetero atoms on the carbon chain are indicated by numerals in accordance with lowest set of locant rule.

(i) 

5 – Ethyl – 3 – azaheptane

(ii) 

2,5,8 – Trioxanonane

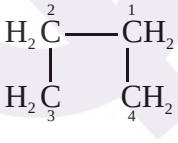
(iii) 

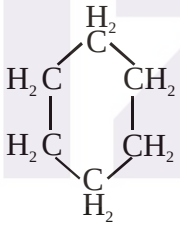
Thiacyclohexane

IUPAC NOMENCLATURE OF ALICYCLIC COMPOUNDS

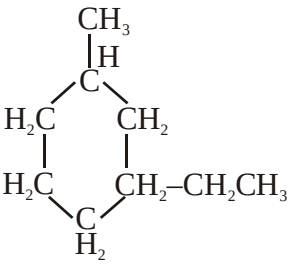
1. Cycloalkanes

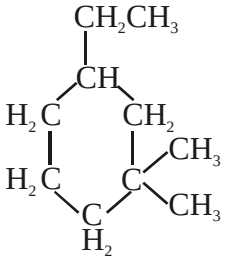
In cycloalkanes, carbon atoms are arranged in a ring.





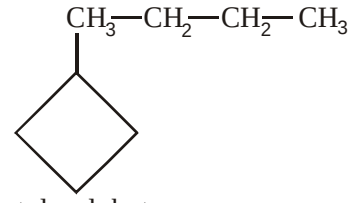
Substituted cycloalkanes are named as alkyl cycloalkanes. The substituent which comes first in the phabetical order is given the lowest possible number provided it does not violet the lowest set of locants rule.





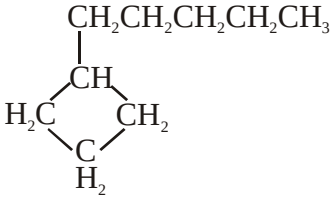
1-Ethyl-3-methylcyclohexane 3-Ethyl-1,1-dimethylcyclohexane

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



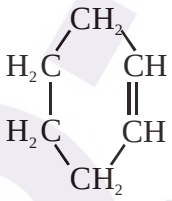
Butylcyclobutane

In case the diphatic chain contains greater number of carbon atoms than present in the ring, the compound is considered as derivative of alkane and the ring is designated as substituent.

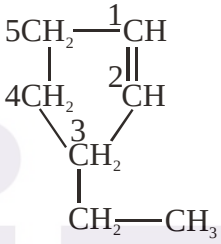


1-Cyclobutylpentane

2. Cycloalkenes and Cycloalkynes :

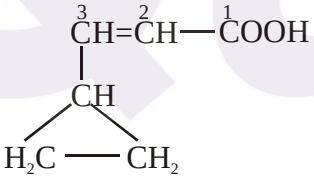


Cyclohexene

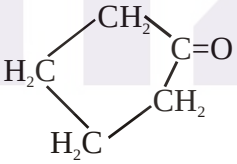


3-Ethylcyclopentene

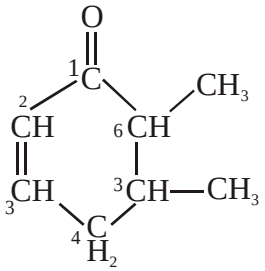
3. Alicyclic compounds containing functional group



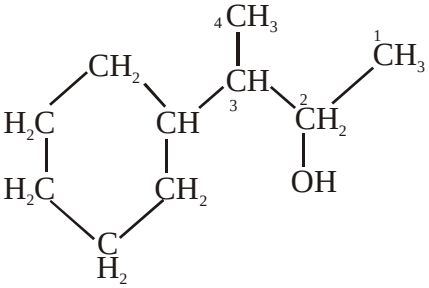
3-cyclopropylprop-2-en-1-oic acid



Cyclopentanone



5,6-Dimethylcyclohex-2-en-1-one



3-Cyclohexylbutan-2-ol

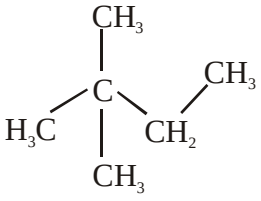
Note : If the side chain contains a multiple bond or a functional group, the alicyclic ring is treated as substitutent irrespective of the size of the ring.

IUPAC Nomenclature of Organic Compounds in Bond Line Structures

The structure of the compound is represented by bond line. The free end is occupied by C-atom group and bent portion is occupied by $-CH_2$ group. C-atom. Rest valency of carbon is satisfied by adding H-atom.

(i)

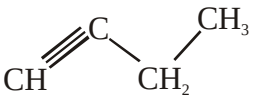




2,2-Dimethylbutane

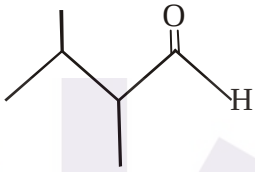
(ii)

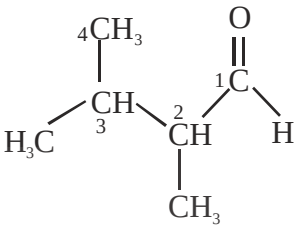




But-1-yne

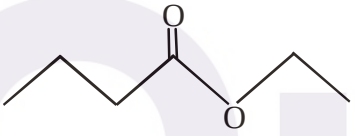
(iii)

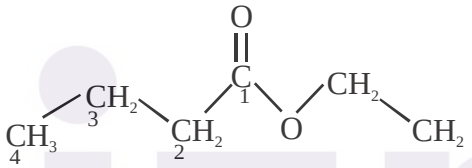




2,2-Dimethylbutanal

(iv)

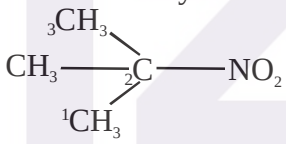




Ethylbutanoate

(v)





2-Methyl-2-nitropropane