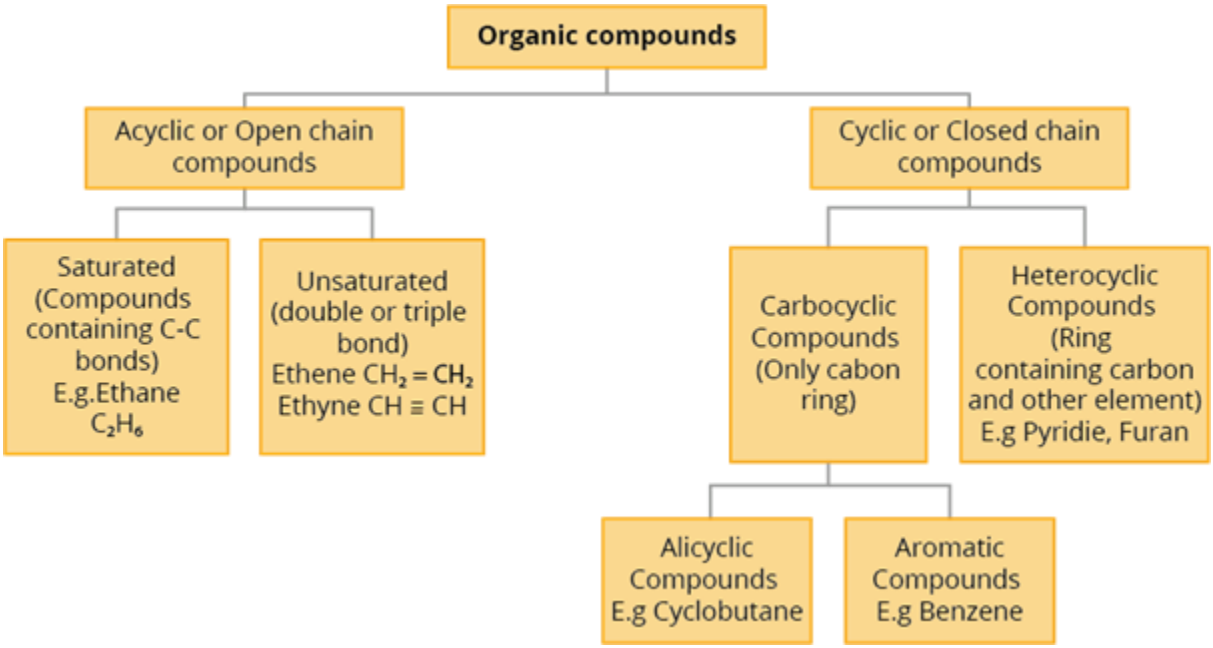
Chapter – 4 Nomenclatures of Organic Systems

4.1 CLASSIFICATION OF ORGANIC COMPOUNDS

The ability of carbon to combine with large number of elements especially O, N, S, X etc, to undergo catenation to form chains of varying lengths and shapes and existence of isomers has led to the formation of more than five million organic compounds. These have been classified into the following main groups.



4.2 TYPE OF ORGANIC COMPOUNDS

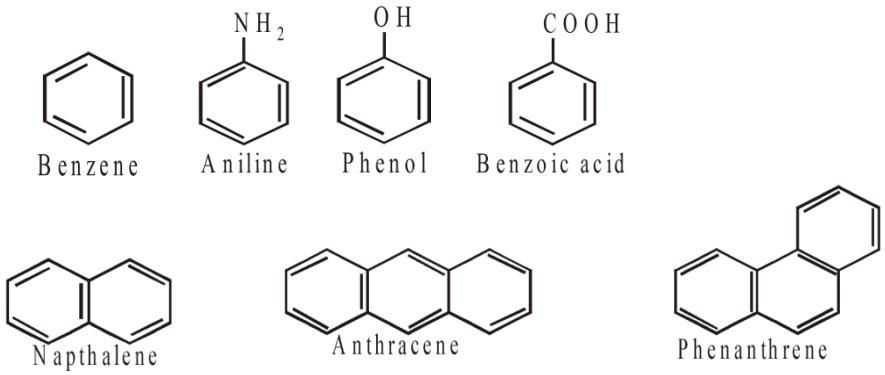
1. ACYCLIC OR OPEN CHAIN COMPOUNDS

2. CYCLIC OR CLOSED CHAIN COMPOUNDS

3. HOMOCYCLIC COMPOUNDS

The ring system is made up of one type of atoms generally carbon.

- **Alicyclic:** The cyclic compounds resembling open chain aliphatic compounds. For example: Cycloalkanes
- **Aromatic:** The benzene, naphthalene and their derivatives etc are homocyclic aromatic compounds

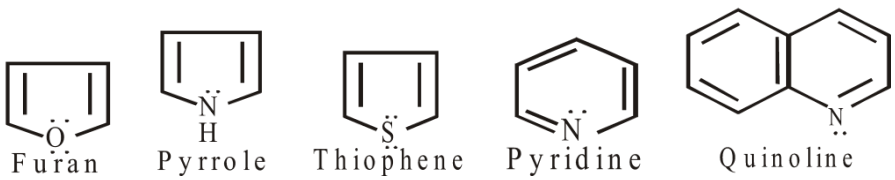


4. HETEROCYCLIC COMPOUNDS

The ring system is made up of two or more than two types of atoms. They may be

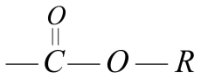
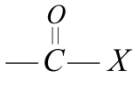
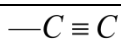
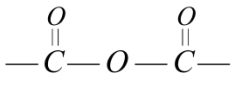
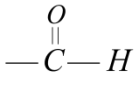
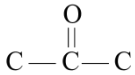
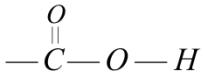
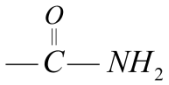
- **Alicyclic:**

- **Aromatic:**



4.3 CLASSIFICATION BASED ON FUNCTIONAL GROUPS

On the basis of functional groups which confer characteristic properties on them, the organic compounds have been classified as follows:

S. No.	Class	Functional group
1.	Halides	X (Cl, Br, I) Halo
2.	Esters	
3.	Olefins Alkenes	>C = C<
4.	Acid halides	
5.	Acetylenes/ Alkynes	
6.	Anhydrides	
7.	Alcohols	—OH (Hydroxy)
8.	Amines	—NH_2
9.	Aldehydes	
10.	Ketones	
11.	Sulphonic acid	—SO_3H
12.	Acids	
13.	Amides	

4.4 HOMOLOGOUS SERIES

A group of a particular class of compounds where a preceding or succeeding member differ by one –CH_2. The members of the series are known as homologues. The homologues

- have the same general formula C_nH_{2n+2} or C_nH_{2n+1} . X
- molecular weight differing by 14 of two successive members.
- can be prepared by general methods of preparation.

- have almost similar chemical properties
- show regular gradation in physical properties such as mpt, bpt, density etc

4.5 NOMENCLATURE

The most widely accepted and the latest system of naming organic compounds is IUPAC (International Union of Pure and Applied Chemists) system, according to which the name essentially consists of three parts.

WORD ROOT

It indicates the nature of the basic carbon skeleton. From C_1 to C_4 common names have been retained and from C_5 upwards Greek number roots have been used

Chain length	Word root	Chain length	Word root
C_1	Meth-	C_7	Hept-
C_2	Eth-	C_8	Oct-
C_3	Prop-	C_9	Non-
C_4	But-	C_{10}	Dec-
C_5	Pent-	C_{11}	Undec-
C_6	Hex-	C_{12}	Dodec-

The generic word root for any carbon chain is “alk”.

SUFFIX

These are of two types:

PRIMARY SUFFIX

It is added to the word root to designate saturation or unsaturation in a carbon chain

Type of Carbon chain	Primary Suffix	Generic name
Saturated	- ane	Alkane
Unsaturated with one C=C	- ene	Alkene
Unsaturated with one C≡C	- yne	Alkyne

SECONDARY SUFFIX

It is added to indicate the functional group present in the compound. The terminal ‘e’ is dropped, if secondary suffix begins with a vowel (a, e, i, o, u, y) but it is retained if the secondary suffix begins with a consonant.

Functional Group	Secondary Suffix	Generic name
– OH	– ol	Alkanol
– CHO	– al	Alkanal
>C = O	– one	Alkanone
– COOH	– oic acid	Alkanoic acid
– COX	– oyl halide	Alkanoyl halide
– $CONH_2$	– amide	Alkanamide
– COOR	– alkyl -- – oate	Alkyl alkanoate
– $(CO)_2O$	– oic anhydride	Alkanoic anhydride
– CN	– nitrile	Alkane nitrile
– SH	– thiol	Alkanethiol
– NH_2	– amine	Alkanamine

PREFIX

They are of two types

PRIMARY PREFIX

It is for cyclic nature of the compound and primary prefix cyclo is used immediately before the word root. eg.:

Primary prefix	Word root	Prim. suffix	Sec. suffix	IUPAC name
Cyclo	hex	ane	–	Cyclohexane

SECONDARY PREFIX

The certain atoms and groups which are not considered as functional groups but are treated as substituents are called secondary prefixes. They are added before the word root in case of acyclic compounds and before the primary prefix in case of cyclic compounds in alphabetical order.

The important secondary prefixes are:

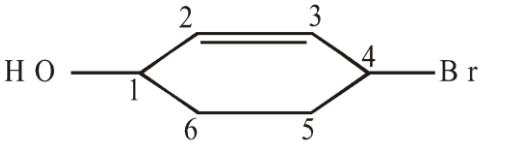
Substituent	Sec. prefix
– X (F, Cl, Br, I)	Halo
– NO_2	Nitro
– NO Nitroso	

$-\overset{+}{N} \equiv \overset{..}{N}$	Diazo
• OR $\left(\begin{matrix}R = \\ CH_3, C_2H_5, C_3H_7, \text{etc.}\end{matrix}\right)$	Alkoxy
–R (CH_3, C_2H_5, C_3H_7, etc)	Alkyl

Thus the complete IUPAC name of an organic compound consists of the following parts

- Secondary prefix
- Primary prefix
- Word root
- Primary suffix
- Secondary suffix

For example:



4-Bromo-cyclo-Hex-2-ene-1-ol

IUPAC name is 4-Bromocyclohex-2-ene-1-ol or 4-Bromo-2-Cyclohexenol

Primary prefix = Cyclo

Secondary prefix = 4-bromo

Word root = hex

Primary suffix = ene

Secondary suffix = ol

4.6 ALKYL GROUPS

Univalent groups formed by the removal of one hydrogen atom from an alkane are known as alkyl groups or alphyl groups. Their names are obtained by changing the suffix **–ane** of parent hydrocarbon by **–yl**.

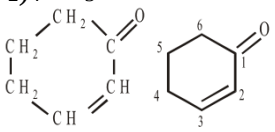
Alkane	**Group**	**Shorthand notation**	**IUPAC Name**
Methane	Methyl CH_3–	Me	Methyl
Ethane	ethyl C_2H_5–	Et	Ethyl

Propane	n-propyl $CH_3CH_2CH_2$– Isopropyl $CH_3-\underset{\vert}{C}H-CH_3$	n-P_r, Iso- P_r	1-propyl 2-propyl
Butane	n-butyl CH_3CH_2–CH_2–CH_2– s-butyl $CH_3CH_2-\underset{\vert}{C}H-CH_3$ Iso-butyl $(CH_3)_2CH$–CH_2– t-butyl $(CH_3)_3C$–	–n-Bu, s-Bu, Iso-Bu, t-Bu,	1-butyl 1-methyl propyl 2-methyl propyl 1,1-dimethyl ethyl

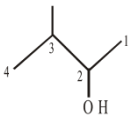
4.7 LINE ANGLE FORMULA

Bonds are represented by lines, carbon atoms are assumed to be present at the start and finish of a line. Nitrogen, oxygen and halogens are labelled, but hydrogens are only shown when bonded to a drawn atom. Each atom is assumed to have sufficient hydrogen atoms around it to make it neutral. For example:

n-Hexane $CH_3(CH_2)_4CH_3$ 

2-Cyclohexenone 

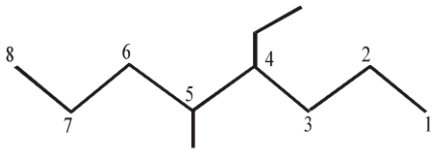
But-1, 3-diene $CH_2=CH-CH=CH_2$ 

3-methyl but-2-ol $CH_3-\underset{\vert}{C}H-\underset{\vert}{C}H-CH_3$ (OH, CH_3) 

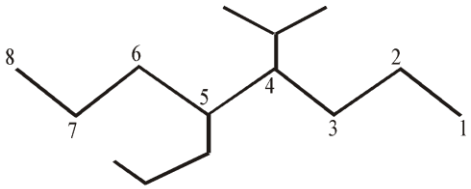
4.8 NOMENCLATURE OF COMPLEX HYDROCARBONS

The following rules are followed:

- **Longest chain rule:** The longest continuous chain of carbon atoms is picked up which forms the base name of the compound.
- **Numbering:** The longest chain is numbered by arabic numerals beginning with the end nearest a substituent.
- If two or more side chains are in equivalent positions, then the one cited first in the name is assigned the lower number.

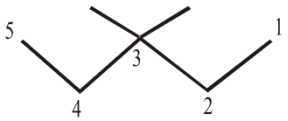


4-Ethyl-5-methyloctane
(not 4-Methyl-5-ethyloctane)



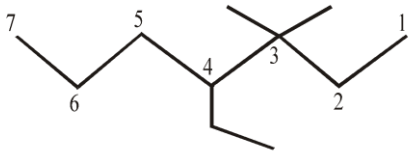
4-isopropyl-5-propyl octane
(not 5-Isopropyl-4-propyloctane)

- If two or more of the same alkyl groups are present, use the prefixes di, tri etc to avoid repetition.



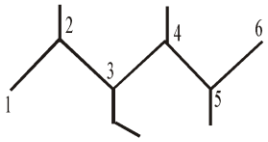
3, 3-Dimethylpentane

- **Alphabetical order**: The side chains are cited in alphabetical order.



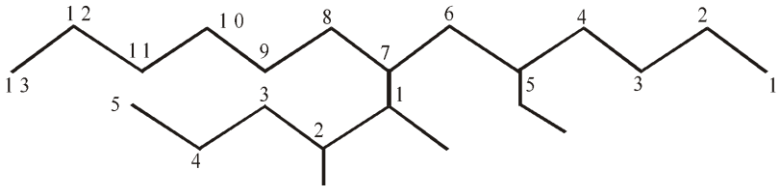
4-Ethyl-3, 3-dimethylheptane

- **Longest chain with maximum number of side chains**: If two or more chains of the same length are possible, choose the one with maximum number of side chains.



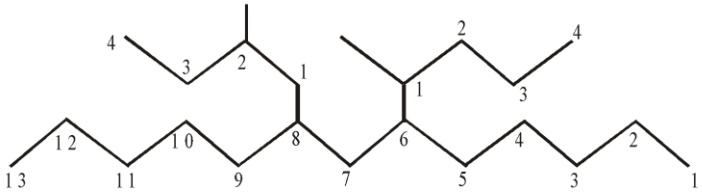
3-Ethyl-2,4,5-trimethylhexane
(not 4-Isopropyl-2,3-dimethylhexane)
(not 3-Isopropyl-4,5-dimethylhexane)

- The name of a complex radical is considered to begin with the first letter of its complete name i.e. including the numerical affix (di, tri, tetra etc are numerical affix) for alphabetical order.



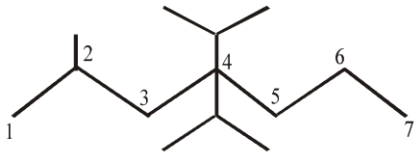
7-(1,2-Dimethyl pentyl)-5-ethyl tridecane

- When the side chains have the identical name the priority is given to side chain having lowest locant



6-(1-Methylbutyl)-8-(2-methyl butyl) tridecane
(not 6-(2-Methylbutyl)-8-(1-Methylbutyl) tridecane)

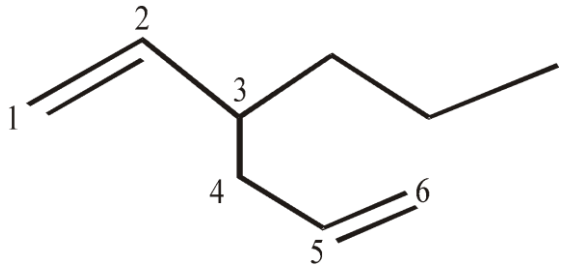
- The numerical prefixes bis, tris tetrakis are used to indicate the multiplicity of substituted substituent



2-Methyl-4-bis(1-methylethyl)heptane

4.9 NOMENCLATURE OF COMPLEX ALKENES AND ALKYNES

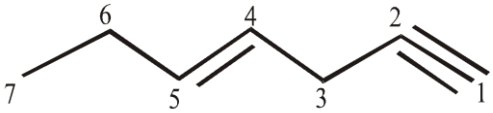
Selection of longest chain containing maximum number of double or triple bonds (sometimes longest chain rule is violated)



3-n-propylhexa-1,5-diene

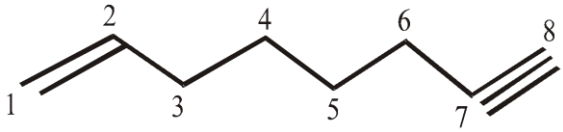
It contains longest chain of 7C atoms, but both the double bonds are not included. Hence longest chain of 6C catoms is picked up)

- If both, the double and triple bonds, are present the compound is regarded as derivative of alkyne. In such cases the terminal 'e' of -ene is dropped if it is followed by suffix starting with a,i,o,u,y. For example :



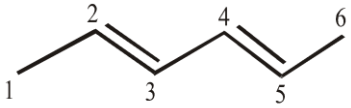
Hept-4-en-1-yne
(not Hept-4-ene-1-yne)

- If double and triple bonds are at equidistant from either side, the preference is given to double bond.

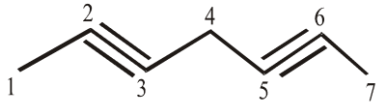


oct-1-en-7-yne
(not oct-7-en-1-yne)

- If the compound contains two or more double or triple bonds a terminal "a" is added to the word root.

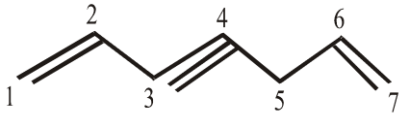


Hexa-2,4-diene
(not Hex-2,4-diene)

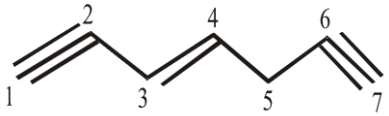


Hepta-2,5-diyne
(not Hept-2,5-diyne)

- The terminal 'a' is not added to the word root when the complete primary suffix do not start with a numerical affix



Hepta-1,6-dien-3-yne



Hept-3-ene-1,6-diyne

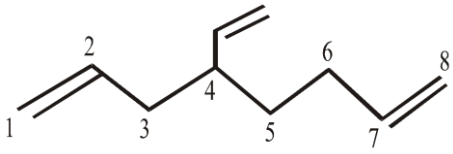
(Note that di, tri, tetra.. are numerical affix)

- Side chains containing multiple bonds are named as follows

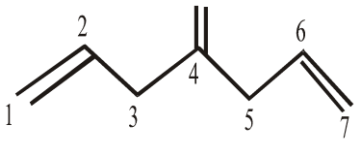
Allyl CH_2= CH_2=CH–CH_2–

Ethylidene CH_3–CH=

Vinyl CH_2=CH–



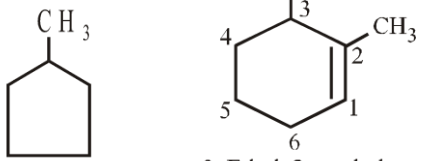
4-Vinylocta-1,7-diene



4-Methylidenhepta-1,6-diene

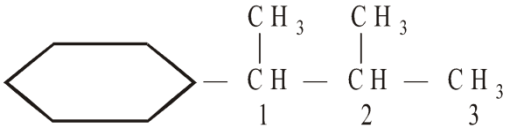
4.10 NOMENCLATURE OF CYCLOALKANES (ALICYCLIC COMPOUNDS)

- The base name is decided by the number of carbon atoms which the cyclic or acyclic portion contains. If the ring contains more or equal number of carbon atoms as alkyl then it is regarded as derivative of cycloalkane
- Carbons are numbered to give lowest numbers to substituted carbons. For example



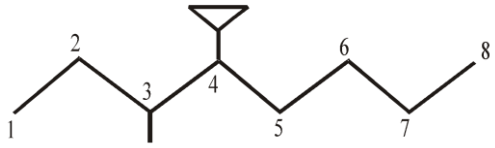
methyl cyclo pentane

3–Ethyl–2–methyl cyclohex-1-ene



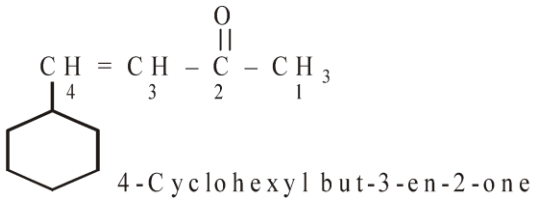
(1, 2-dimethyl propyl) cyclohexane

- When there are more acyclic than cyclic carbons the cyclic part becomes cycloalkyl substituent



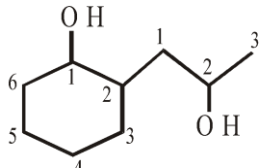
4-Cyclopropyl-3-methyloctane

- When acyclic portion contains a multiple bond or a functional group, the cyclic portion is treated as substituent.



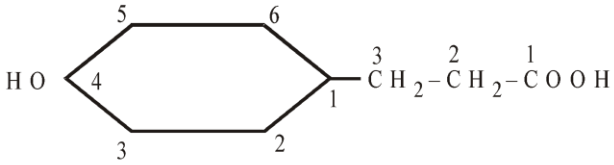
4-Cyclohexyl but-3-en-2-one

- In case when both contain the same functional group, the base name is decided by the number of c-atoms.



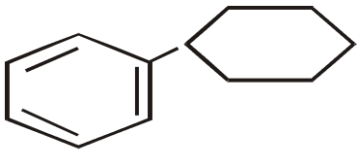
2-(2-Hydroxypropyl) cyclohexan-1-ol

- When both contain the different functional groups, the base name is decided by principal characteristic group



3-(4-Hydroxycyclohexyl)propanoic acid

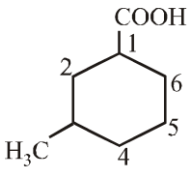
- When the acylic ring is directly attached to benzene ring, it is named as derivative of benzene



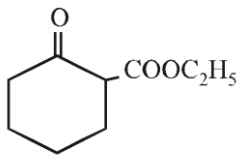
Cyclohexyl benzene

- Presence of certain groups

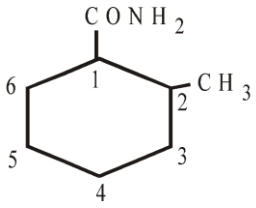
Functional gp.	**Suffix**
–COOH	Carboxylic acid
–COOR	Alkyl carboxylate
–COX	Carbonyl halide
$-CONH_2$	Carboxamide
$-C \equiv N$	Carbonitrile
–CHO	Carbaldehyde



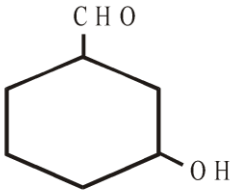
3-Methyl Cyclohexane Carboxylic acid



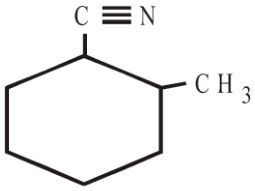
Ethyl 2-Oxo, cyclohexane 1-carboxylate



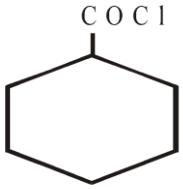
2-Methylcyclohexane-1-carboxamide



3-hydroxy cyclohexane carbaldehyde



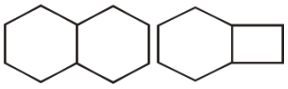
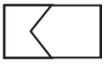
2-Methyl cyclohexane carbonitrile



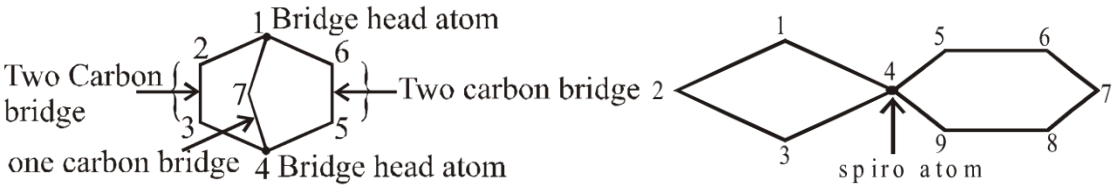
cyclohexane-1-carbonyl chloride

4.11 NOMENCLATURE OF POLYCYCLIC ALKANES

There are three ways that rings can be joined.

- Fused rings 
- Bridged rings 
- Spirocyclic compounds 

The carbon atoms common to both the rings are called **bridge head atoms**. The chain of carbon atoms connecting the bridge head atoms is called a **bridge**.

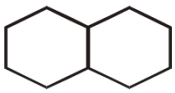


Numbering of C-atoms in fused rings and bridge rings: The numbering starts from bridge head carbon, proceeds along the longest bridge passing through the second bridge head atom, proceeds to the next longest bridge and completed along the shortest path.

Numbering of C-atoms in spiro compounds: The numbering starts from the carbon atom, next to spiro atom, present in the smaller ring giving minimum number to atoms containing functional groups.

FUSED RINGS

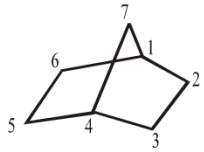
Fused rings share two adjacent carbon atoms and the bond between them eg. :



Bicyclo [4.4.0]decane

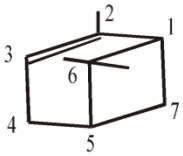
BRIDGED RINGS

These share two non adjacent carbon atoms (the bridge head carbons) and one or more carbon atoms between them

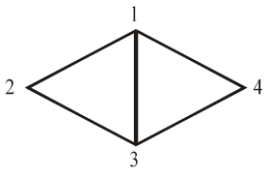


Bicyclo [2.2.1]heptane

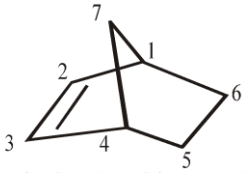
More examples of bridge Compounds



2, 6, 6-Trimethyl bicyclo[3.1.1]hept-2-ene



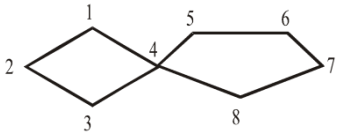
Bicyclo [1.1.0] butane



Bicyclo[2.2.1]hept-2-ene

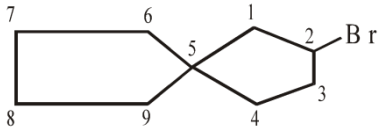
SPIROCYCLIC COMPOUNDS

The two rings share one carbon atom

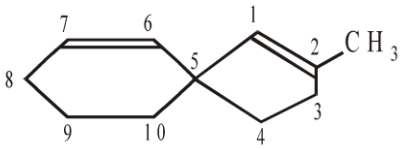


Spiro [4.3] octane

More examples of spiro Compounds



2-Bromo spiro[4.4] nonane

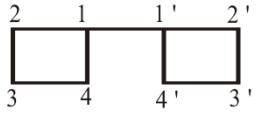


2-methyl spiro[4.5]deca-1, 6-diene

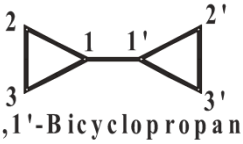
4.12 NOMENCLATURE OF COMPOUNDS CONTAINING IDENTICAL CYCLIC UNITS JOINED BY A SINGLE BOND

No. of cyclic hydrocarbon units	Two	Three	Four
Prefix	bu	ter	quarter

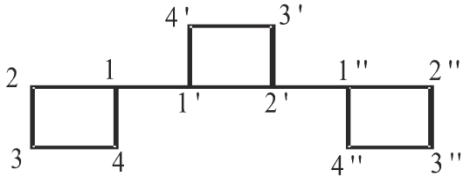
Numbering of C-atoms: The numbering starts from the C-atom joining the rings.



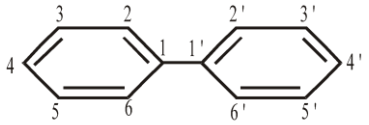
1,1'-Bicyclobutane



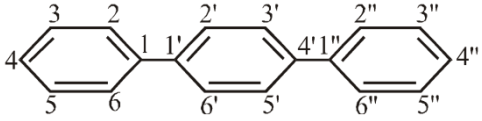
1,1'-Bicyclopropane



1,1',2',1''-Tercyclobutane



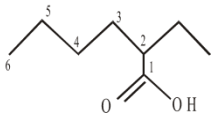
1,1'-Biphenyl



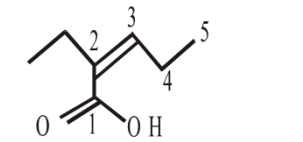
1,1',4',1''-Terphenyl

4.13 NOMENCLATURE OF COMPOUNDS CONTAINING TERMINATING FUNCTIONAL GROUPS

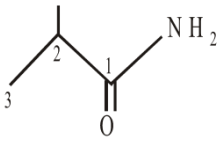
If only one group such as –COOH, –CHO, –COOR, –$CONH_2$, –COCl or – is present in the molecule it is always given number 1 and 1 is never written when there is no ambiguity.



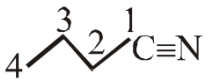
2-Ethylhexanoic acid



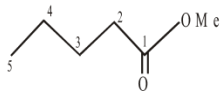
2-Ethylpent-2-enoic acid



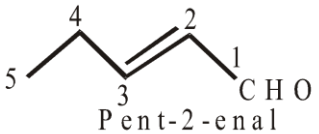
2-Methylpropanamide



Butane nitrile
(e is retained as it comes before n)



Methylpentanoate

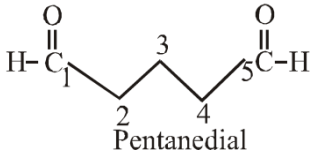


Pent-2-enal
(terminal e of ene is removed as it comes before a)

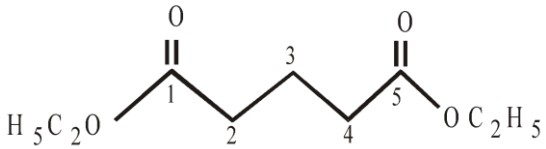
4.13 NOMENCLATURE OF COMPOUNDS CONTAINING TWO OR MORE THAN TWO SIMILAR TERMINAL GROUPS

PRESENCE OF ONLY TWO SIMILAR TERMINAL GROUPS

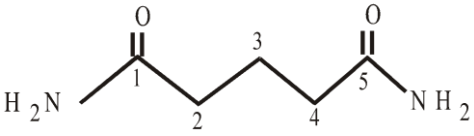
The carbon atoms of such groups are included in the principal chain. For example



Pentanedial



Diethyl pentanedioate



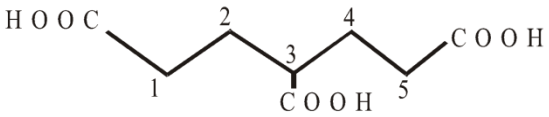
Pentanediamide

PRESENCE OF MORE THAN TWO SIMILAR TERMINAL GROUPS ATTACHED TO THE MAIN PRINCIPAL CHAIN

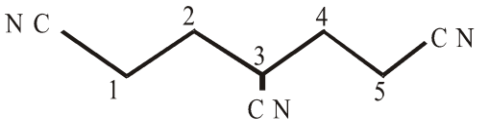
In this case special suffixes are used and carbons of terminal groups are not counted in the principal chain

Functional groups	Suffix
–COOH	- Carboxylic acid
–CHO	- Carbaldehyde
–COX	- Carbonylhalide

$-CONH_2$	- Carboxamide
–COOR	- Alkyl carboxylate
–CN	- Carbonitrile



Pentane-1,3,5-tricarboxylic acid



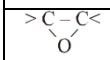
Pentane-1,3,5-tricarbonitrile

4.13 NOMENCLATURE OF COMPOUNDS CONTAINING MORE THAN ONE TYPE OF FUNCTIONAL GROUPS

In such case the compound is regarded as derivative of senior functional group and the other functional groups are regarded as substituents. The numbering of the parent chain is done in such a way so that the functional group of highest priority gets the lower number and the chain contains the maximum number of functional groups.

The seniority of functional groups (highest priority) follow the following order:-

Group	**Prefix name**	**2º Suffix name**
$-SO_3H$	Sulpho	Sulphonic acid
– COOH	Carboxy	Oic acid
– COOR	alkoxy carbonyl	Oate
– COX	Halo carbonyl/Halo formyl	–oyl halide
$-CONH_2$	Carbamoyl	amide
– CHO	Aldo or formyl	al
– CN	Cyano	nitrile
– NC	Isocyano	Isonitrile
>C = O	Keto or oxo	one
– OH	Hydroxy	ol

– SH	Mercapto	thiol
– NH_2	Amino	Amine
– OR	Alkoxy	–
	Epoxy	–
> C = C <	–	ene
$-C \equiv C-$	–	yne
– N = N	Azo	–
– NO_2	Nitro	–
– NO	Nitroso	–
– X (Cl, Br, I)	Halo (Cl, Br, I)	

The terminal e of the primary suffix is replaced by the suffix name of functional group.

Alphabetical order for substituents : These should be placed in alphabetical order.

Naming of substituted substituents : In this case the subsidiary substituents are named as prefixes. For example

$-CH_2-CHO$ Formyl methyl $=CH-CH_3$ Ethylidene

$\equiv C-CH_2-CH_3$ Propylidyne $-CH_2-COOH$ Carboxymethyl

$-CH_2Cl$ Chloromethyl $-CH_2-C \equiv N$ Cyanomethyl

$-CH_2-CH_2-CO-NH_2$ Carbomoylethyl

4.14 NOMENCLATURE OF AROMATIC COMPOUNDS

Generally Benzene and its derivatives are known as aromatic compounds. They are of two types

- **Nuclear substituted** : The functional group is directly attached to the benzene nucleus e.g. phenol, toluene, chlorobenzene etc.
- **Side chain substituted** : The functional group is present in the side chain e.g. Benzyl alcohol, Benzylamine etc.

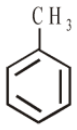
In the first case the compounds are named as derivatives of benzene and in the second case as derivatives of aliphatic compounds (except arenes).

The IUPAC name of benzene is cyclohex-1,3,5-triene, but now aromatic compounds have their popular common name adopted by IUPAC. In IUPAC system the position of functional groups are indicated by arabic numerals i.e. 1, 2, 3 instead of o, m and p.

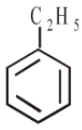
AROMATIC HYDROCARBONS (ARENES)

CONTAINING ONE RING

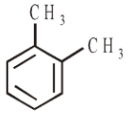
Benzene



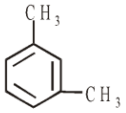
Methyl benzne
(Toluene)



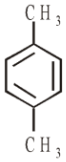
Ethyl benzne



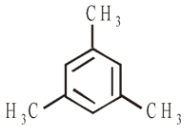
1, 2-dimethylbenzene
(o-xylene)



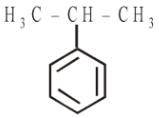
1, 3-dimethylbenzene
(m-xylene)



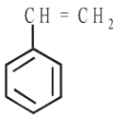
1, 4-dimethylbenzene
(p.xylene)



1, 3, 5-trimethylbenzene
(mesitylene)

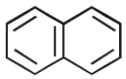


2-propylbenzene
(cummene)

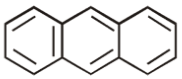


ethenylbenzene
(styrene, vinyl benzene)

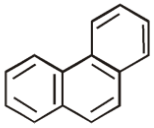
CONTAINING MORE THAN ONE RING



Naphthalene

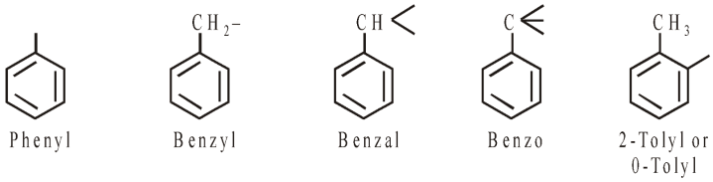


Anthracene

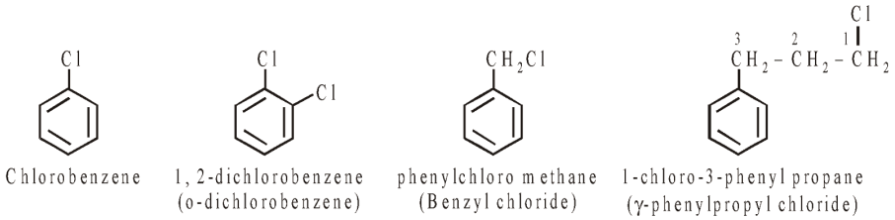


Phenanthrene

ARYL GROUPS

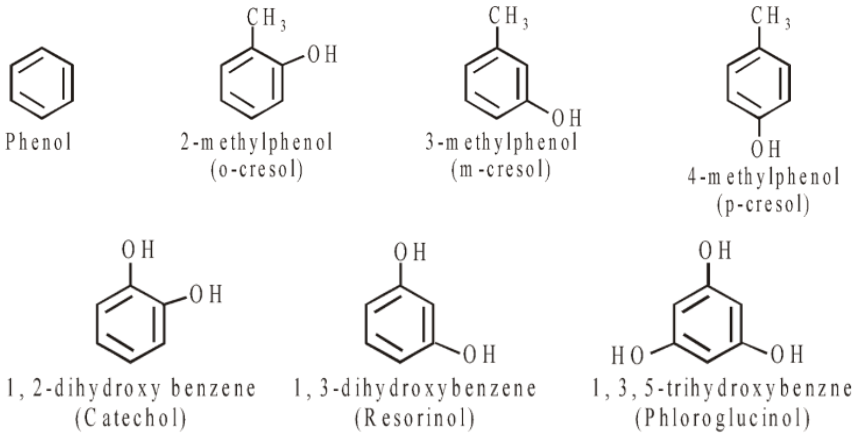


HALOGEN DERIVATIVES

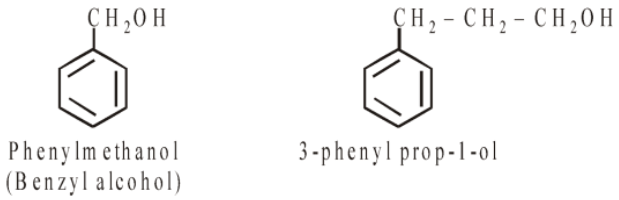


PHENOLS

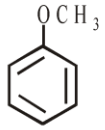
Nuclear substituted hydroxy derivatives are known as phenols

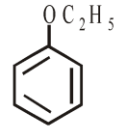


Side chain substituted hydroxy derivatives are known as alcohols

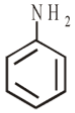


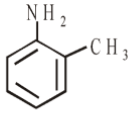
AROMATIC ETHERS

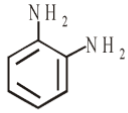

Methoxybenzene
(Anisole)


Ethoxybenzene
(phenetole)

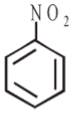
AMINES

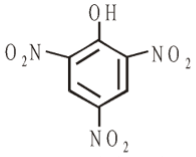

Benzenamine
(Aniline)

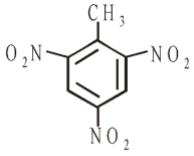

2-methylbenzenamine
(o-Toluidine)


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

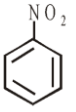
NITRO COMPOUNDS

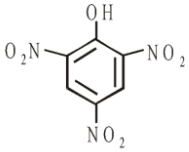

Nitro benzene

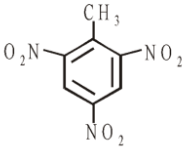

2, 4, 6-trinitrophenol
(Picric acid)


2, 4, 6-trinitrotoluene
(T.N.T.)

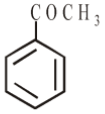
ALDEHYDES

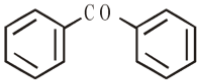

Nitro benzene


2, 4, 6-trinitrophenol
(Picric acid)

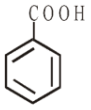

2, 4, 6-trinitrotoluene
(T.N.T.)

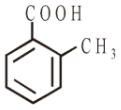
KETONES

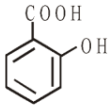

Methyl phenyl Ketone
(Acetophenone)

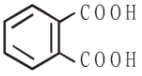

Diphenyl Ketone
(Benzophenone)

ACIDS

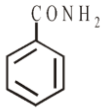

Benzoic acid


2-methylbenzoic acid
(o-Toluic acid)

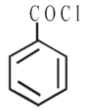

2-Hydroxybenzoic acid
(Salicylic acid)


Benzene-1, 2-dicarboxylic acid
(Phthalic acid)

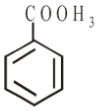
ACID DERIVATIVES



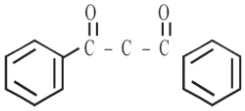
Benzamide



Benzoyl chloride

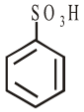


Methyl benzoate



Benzoic anhydride

SULPHONIC ACIDS



Benzene sulphonic acid