Chapter 01 Classification and Nomenclature

CONTENT

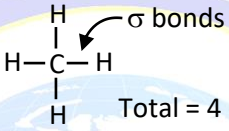
Bonding in organic compounds

Two types of covalent bond exist in organic compounds.

(a) sigma bond (σ): the covalent bond formed between 2 atoms by mutual sharing of 1 pair of e–.

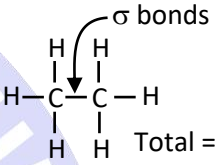
It is denoted by (–).

Ex. In CH_4 Molecule



Total = 4 σ bonds

In C_2H_6 Molecule



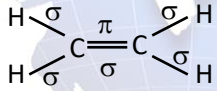
Total = 7 σ bonds

(b) Multiple bond: A multiple bond is a chemical bond where two or more electron pairs are shared between two atoms.

It is denoted by (= or ≡).

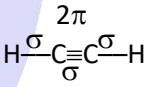
Example

(i) In ethene molecule



Total σ = 5
π = 1

(ii) In ethyne molecule



Total σ = 3
π = 2

Example: Calculate σ and π bond in following compounds.

(a) $HC\equiv C–CH=CH–CH_3$ (b) $CH_2=C=CH–CH_3$

Solution: (a) σ_{C-C} : 4 ; σ_{C-H} : 6 ; $\pi_{C=C}$: 1 ; $\pi_{C\equiv C}$: 2

(b) σ_{C-C} : 3 ; σ_{C-H} : 6 ; $\pi_{C=C}$: 2

Some important definitions:

(i) Catenation: The property of atoms of an element to link with one another forming chains of identical atoms is called catenation.

(ii) Homologous series: Homologous series may be defined as a series of similar constituted compounds in which the members possess the same functional group, have similar chemical characteristics and have a regular gradation in their physical properties. The two consecutive members differ in their molecular formula by CH_2.

Structural representation of organic compounds

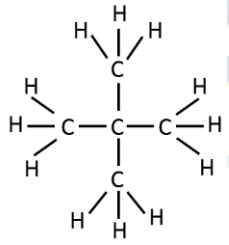
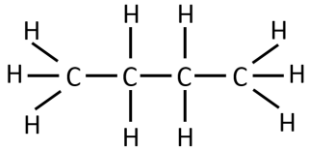
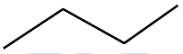
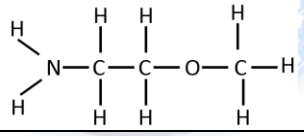
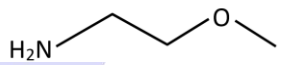
There are three ways for representation of organic compounds:

(i) Complete structural formula: – Such a structural formula focuses on the electrons involved in bond formation. A single dash (–) represents a single bond, double dash (=) is used for double bond and a

triple dash (≡) represents triple bond. Lone-pairs of electrons on heteroatoms (e.g., oxygen, nitrogen, sulphur, halogens etc.) may or may not be shown.

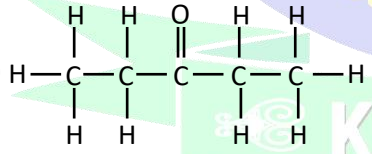
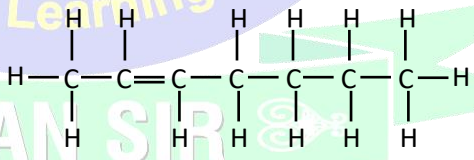
(ii) Condensed structural formula : Structural formulas can be further abbreviated by omitting some or all of the dashes representing covalent bonds and by indicating the number of identical groups attached to an atom by a subscript. The resulting expression of the compounds is called a condensed structural formula.

(iii) Bond line formula:- In this formula, carbon and hydrogen atoms are not shown and the lines representing carbon -carbon bonds are drawn in a zig-zag fashion. The only atoms specially written are oxygen chlorine, nitrogen etc.

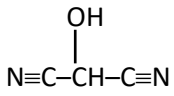
Condensed form	Expanded form	Bond line form
$C(CH_3)_4$		
$CH_3(CH_2)_2CH_3$		
$NH_2–CH_2–CH_2–O–CH_3$		

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

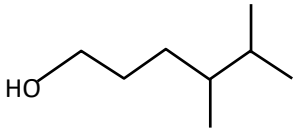
(a) $CH_3CH_2COCH_2CH_3$ **(b)** $CH_3CH=CH(CH_2)_3CH_3$

Solution: **(a)**  **(b)** 

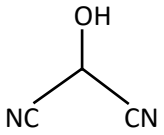
Example For each of the following compounds, write a condensed formula and also their bond-line formula.

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

Solution: Condensed formula: Bond-line formula:

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

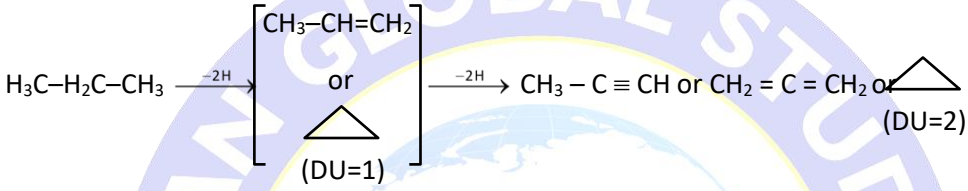
(b) $HOCH(CN)_2$



Degree of Unsaturation (DU)

The presence of double bonds or rings within a molecule is indicated by a quantity called degree of unsaturation **Applications:** To identify the no. of π bonds or ring and also helpful in determining the structure of the molecule.

D3: Definition: Deficiency of 2H atoms with respect to fully saturated acyclic hydrocarbon is equivalent to One DU. It is also known as Hydrogen Deficiency Index (HDI) or Double Bond Equivalence (DBE)



$$\text{Degree of unsaturation (D.U.)} = \frac{(2n+2)-(\text{No.of H atom + No. of X atoms} - \text{No. of N atoms})}{2}$$

Where n = number of carbon atoms in the molecule

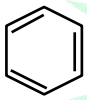
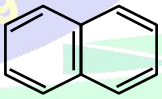
Note: Total no. of cyclic rings + double bonds will give us degree of unsaturation.

One double bond = one DU

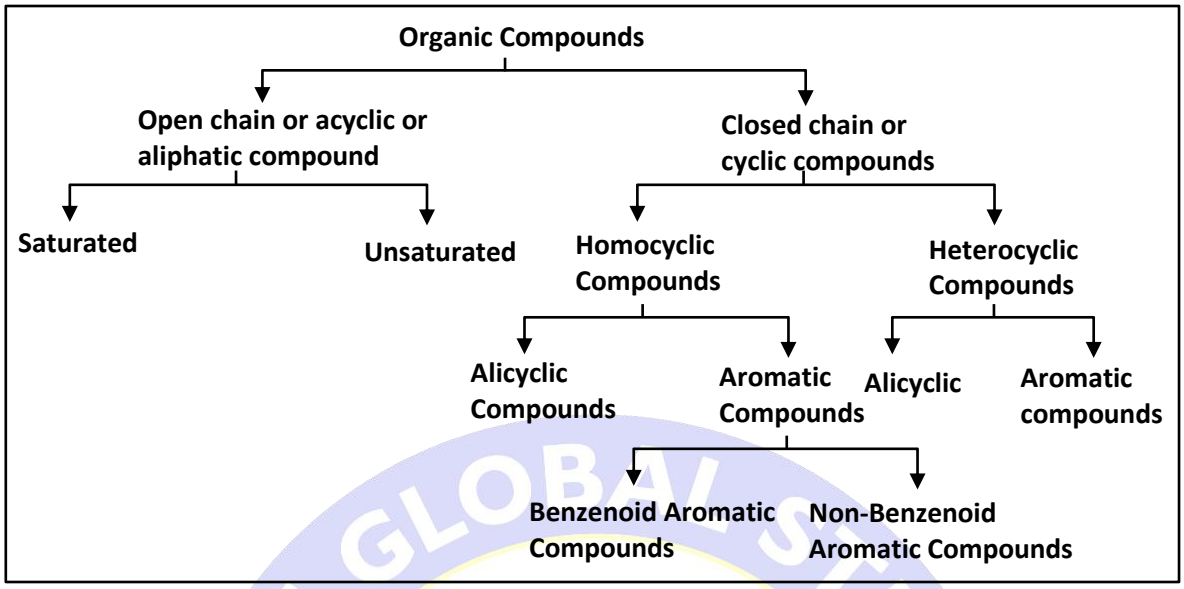
One ring = one DU

One triple bond = two DU

Ex. (i) $CH_2 = CH_2$ $\quad DU = \frac{(2\times2+2)-4}{2} = 2/2 = 1$ (ii)  DU=2

(iii)  DU=4 (iv)  DU=7

Classification of organic compounds



Organic compounds and functional groups

Number of known organic compounds is much more than inorganic compounds but, it has been possible to group them into classes or families bases on their structural features. This has given organic chemistry a logical and systematic shape. Examples are as follows:

1. Alkanes [general formula C_nH_{2n+2} where n = 1, 2, 3……]

These are open-chain aliphatic saturated hydrocarbon which have no functional groups. These are also called paraffins.

n = 1	$\Rightarrow CH_4$	–	Methane	n = 2	$\Rightarrow C_2H_6$	–	Ethane
n = 3	$\Rightarrow CH_3CH_2CH_3$	–	Propane	n = 4	$\Rightarrow CH_3CH_2CH_2CH_3$	–	Butane
n = 5	$\Rightarrow CH_3CH_2CH_2CH_2CH_3$	–	Pentane	n = 10	$\Rightarrow CH_3(CH_2)_8CH_3$	–	Decane

2. Alkenes [general formula C_nH_{2n} where n = 2, 3, ……]

Alkenes are open chain unsaturated hydrocarbons and having carbon–carbon double bonds (C = C). These are also called alkylenes or olefins. The first three members are generally named by their common names.

Ex. $CH_2 = CH_2$ $CH_3 - CH = CH_2$ $CH_3 - CH_2 - CH = CH_2$ $CH_3 - \underset{CH_3}{\underset{|}{C}} = CH_2$

ethylene Propylene butylene Isobutylene

3. Alkynes [general formula C_nH_{2n-2} where n = 2, 3, …….]

Unsaturated aliphatic hydrocarbons containing a carbon–carbon triple bond are called alkynes. The common names of a few simple alkynes are given below.

$CH \equiv CH$	–	Acetylene
$CH_3 - C \equiv CH$	–	Methyl acetylene
$CH_3 - CH_2 - C \equiv CH$	–	Ethyl acetylene

$CH_3–C\equiv C–CH(CH_3)_2$ – Methyl isopropyl acetylene

4. Some names of hydrocarbon groups

(A) Alkyl, Alkenyl & Alkynyl groups

Alkane (C_nH_{2n+2}) $\xrightarrow{-H}$ Alk + yl (C_nH_{2n+1})

Alkene (C_nH_{2n}) $\xrightarrow{-H}$ Alken + yl (C_nH_{2n-1})

Alkyne (C_nH_{2n-2}) $\xrightarrow{-H}$ Alkyn + yl (C_nH_{2n-3})

Ex. Methane $\xrightarrow[+yl]{-ane}$ methyl $\left(CH_4 \xrightarrow{-H} -CH_3\right)$

Propane $\xrightarrow[+yl]{-ane}$ propyl $\left(C_3H_8 \xrightarrow{-H} -C_3H_7\right)$

$CH_2 = CH_2 \xrightarrow{\text{remove H}} -CH=CH_2$ (vinyl group)/ethenyl.

$CH_2 = \overset{1}{CH} - \overset{2}{CH_3} \overset{3}{}$

remove H from C_3 → $CH_2 = CH – CH_2 –$ allyl group

remove H from C_2 → $CH_2 = \underset{\displaystyle CH_3}{\overset{\displaystyle |}{C}}–$ Isopropenyl group

$HC\equiv CH \xrightarrow{-H}$ $HC \equiv C –$ (Ethynyl)

$H_3C–C\equiv CH \xrightarrow{-H}$ $H_3C–C\equiv C–$ (propynyl)

(B) Iso alkyl group: A compound having $\underset{\displaystyle CH_3}{\overset{\displaystyle |}{CH}} – CH_3$ groups is called iso alkyl group.

$CH_3 – \underset{\displaystyle CH_3}{\overset{\displaystyle |}{CH}} –$ Iso propyl

$CH_3 – \underset{\displaystyle CH_3}{\overset{\displaystyle |}{CH}} – CH_2 –$ Iso butyl

$CH_3 – \underset{\displaystyle CH_3}{\overset{\displaystyle |}{CH}} – CH_2 – CH_2 –$ Isopentyl

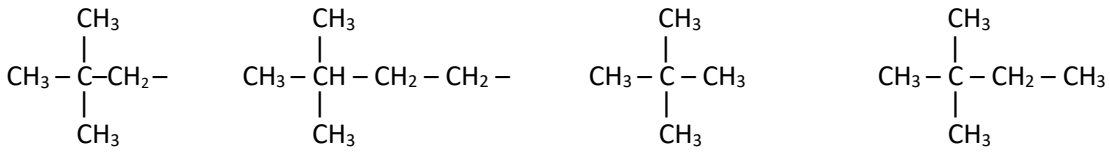
$CH_3 – \underset{\displaystyle CH_3}{\overset{\displaystyle |}{CH}} – CH_2 – CH_3$ Iso pentane

Exception: Iso octane (If standard convention is to be followed, iso octane would be $CH_3–CH(CH_3)–CH_2CH_2CH_2CH_2CH_3$ but 2, 2, 4- trimethyl pentane is by the most important isomer of octane and is so historically, it has been assigned this name.)

$$CH_3 – \underset{\displaystyle CH_3}{\overset{\displaystyle CH_3}{\overset{\displaystyle |}{\overset{\displaystyle |}{C}}}} – CH_2 – \underset{\displaystyle CH_3}{\overset{\displaystyle |}{CH}} – CH_3$$

(C) Neo alkyl group: Compound having $\left(CH_3 – \underset{\displaystyle CH_3}{\overset{\displaystyle CH_3}{\overset{\displaystyle |}{\overset{\displaystyle |}{C}}}} – CH_2 –\right)$ group is called neo alkyl group.

Ex.



Neopentyl Neohexyl Neopentane Neohexane

5. Functional group and residue

The characteristic group of atom which decide the physical and chemical properties of an organic molecule is called functional group.

Functional groups is that portion of molecule which is highly reactive and takes part in chemical reactions. Rest of the molecule is called Residue.

Ex. $\underbrace{CH_3CH_2CH_2CH_2}_{\text{Residue}}-\underbrace{COOH}_{\text{Functional Group}}$

IUPAC system of nomenclature

The IUPAC name of any organic compound consists of maximum five parts in the following sequence.

Secondary prefix + primary prefix + word root + Primary suffix + Secondary suffix

1. Word root:

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

No. of carbon atoms in parent chain	Word root (Alk)	No. of carbon atoms in parent chain	Word root (Alk)	No. of carbon atoms in parent chain	Word root (Alk)
1	Meth	9	Non	20	Icos
2	Eth	10	Dec	30	Triacont
3	Prop	11	Undec	40	Tetracont
4	But	12	Dodec	50	Pentacont
5	Pent	13	Tridec	60	Hexacont
6	Hex	14	Tetradec	70	Heptacont
7	Hept	15	Pentadec	80	Octacont
8	Oct	16	Hexadec	100	Cent & Hect

2. Primary Suffix.

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

Type of carbon chain	Primary suffix	General name
(a) Saturated	– ane	Alkane
(b) Unsaturated with one double bond	– ene	Alkene

(c) Unsaturated with one triple bond	– yne	Alkyne

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

Type of carbon chain	Primary suffix	General name
(a) Unsaturated with two double bonds	(a) + diene	Alkadiene
(b) Unsaturated with two triple bonds	(a) + diyne	Alkadiyne
(c) Both double and triple bonds	enyne	Alkenyne

3. Secondary suffix:

A secondary suffix is than added to the primary suffix to indicate the nature of the functional group present in the organic compounds. Secondary suffix of important functional groups are given below in their decreasing order of seniority (priority).

	Class	Name	Suffix	Prefix
1.	R – COOH	Alkanoic Acid	– oic acid (carboxylic acid)	Carboxy
2.	$R-SO_3H$	Alkane sulphonic Acid	– sulphonic acid	Sulpho
3.	$R-\underset{\underset{O}{\|}}{C}-O-\underset{\underset{O}{\|}}{C}-R$	Alkanonic Anhydride	– oic anhydride (carboxylic anhydride)	----------
4.	R – COOR	Alkyl alkanoate	– oate (carboxylate)	Alkoxy carbonyl or alkanoyl oxy
5.	$R-\underset{\underset{O}{\|}}{C}-X$	Alkanoyl halide	–oyl halide (carbonyl halide)	Halo carbonyl
6.	$R-\underset{\underset{O}{\|}}{C}-NH_2$	Alkanamide	– amide (carboxamide)	Carbamoyl
7.	$R-C\equiv N$	Alkanenitrile	– nitrile (carbonitrile)	cyano
8.	$R-\underset{\underset{O}{\|}}{C}-H$	Alkanal	– al (carbaldehyde)	Formyl / oxo
9.	$R-\underset{\underset{O}{\|}}{C}-R$	Alkanone	– one	oxo
10.	R – OH	Alkanol	– ol	hydroxy
11.	R – SH	Alkanethiol	– thiol	mercapto
12.	$R-NH_2$	Alkanamine	– amine	amino

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

Organic compounds	Word root	Primary suffix	Secondary suffix	IUPAC name
CH_3CH_2OH	Eth	an(e)	ol	Ethanol
$CH_3CH_2CH_2NH_2$	Prop	an(e)	amine	Propanamine

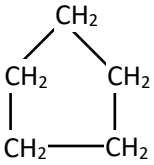
$CH_3CH_2CH_2COOH$	But	an(e)	oic acid	Butanoic acid
CH_3CH_2CN	Prop	an(e)	nitrile	Propanitrile
$CH_2 = CHCHO$	Prop	en(e)	Al	Propenal
$HC \equiv CCOOH$	Prop	yn(e)	oic acid	Propynoic acid

4. Primary prefix:

A primary prefix is used simply to distinguish cyclic from acyclic compounds.

For example, in case of carbocyclic compounds, (cyclic compounds containing only carbon atoms in the ring), a primary prefix, cyclo is used immediately before the word root. Thus,

Ex.



Cyclo	+	pent	+	ane	=	Cyclopentane
Primary prefix		Word root		Primary suffix		IUPAC name

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

5. Secondary prefix:

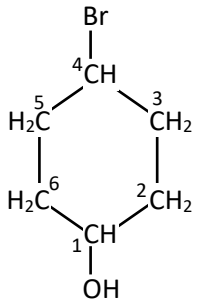
In IUPAC system of nomenclature, certain groups are not considered as functional groups but are treated as substituents. These are called secondary prefixes and are added immediately before the word root (or the primary prefix in case of carbocyclic compounds) in alphabetical order to denote the side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

Substituent group	Secondary prefix	Substituent group	Secondary prefix
– F	Fluoro	$-OCH_3$ (– OMe)	Methoxy
– Cl	Chloro	$-OC_2H_5$(–OEt)	Ethoxy
– Br	Bromo	– R	Alkyl
– I	Iodo	$-CH_3$ (–Me)	Methyl
$-NO_2$	Nitro	$-C_2H_5$ (–Et)	Ethyl
– NO	Nitroso	$-CH_2CH_2CH_3$(n-Pr)	n-Propyl
$-\overset{\oplus}{N} \equiv N$	Diazo	$-CH(CH_3)_2$ (–iPr)	Isopropyl
– OR	Alkoxy	$-C(CH_3)_3$ (t-Bu)	t-Butyl

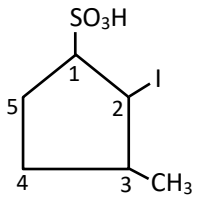
Example:

Organic compounds	Secondary prefix	Word root	Primary	IUPAC name
CH_3CH_2–Br	Bromo	eth	ane	Bromoethane
$CH_3 - NO_2$	Nitro	meth	ane	Nitromethane
$C_2H_5 - OC_2H_5$	Ethoxy	eth	ane	Ethoxyethane

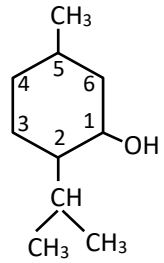
Ex.



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



2-Iodo-3-methyl	+	cyclo	+	pent	+	ane	+	1-sulphonic acid
Secondary prefix		Primary prefix		Word root		Primary suffix		Secondary suffix



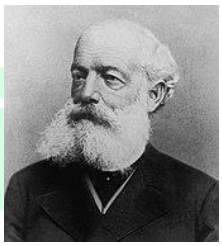
2 – Isopropyl – 5 – methylcyclohexanol

Hence secondary prefix = 2 – Isopropyl – 5 methyl
Primary prefix = cyclo
Word root = hex
Primary suffix = an(e)
Secondary suffix = ol

DETECTIVE MIND

Who started international nomenclature system?????

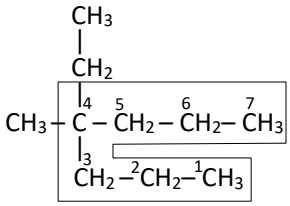
The need for an international standard for chemistry was first addressed in 1860 by a committee headed by German scientist Friedrich August Kekulé von Stradonitz. This committee was the first international conference to create an international naming system for organic compounds.



IUPAC nomenclature of branched / complex alkanes

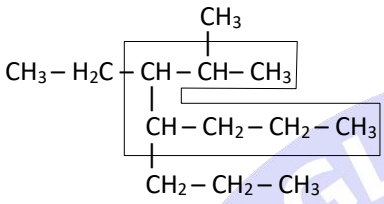
1. parent carbon chain selection:

(a) Select the longest continuous carbon chain in the molecule



Longest chain has 7 carbons so word root is "Hept"

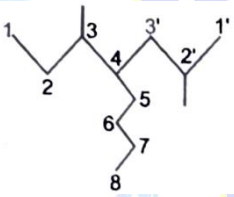
(b) When chains of equal lengths are competing for selection then that chain is selected which has more number substituents/branches.



Longest chain has 7 carbon & 3 substiutents

(c) When the number of substituents are same then the substituents at the nearest positions from the either end is prefer for parent chain selection.

Ex. Here, 2 choices for longest chain



Chain- (A) 1–2–3–4–5–6–7–8

Chain- (B) 1'–2'–3'–4–5–6–7–8

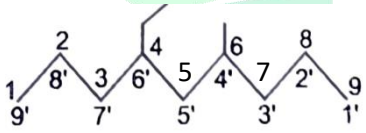
Chain- (A) & Chain- (B) both have 2 substituents but in chain-B substituent is nearer (at 2nd position) than in chain-A (at 3rd position). So Chain-B will be preferred.

(d) If the two substituents are found in equivalent positions the lower number is given to the one coming first in the alphabetical order.

Ex. Here, 2 choices for longest chain

Chain- (A) 1–2–3–4–5–6–7–8–9

Chain- (B) 1'–2'–3'–4'–5'–6'–7'–8'–9'



In both chain-A & chain-B, substituents are at same position (4th). In chain-A substituent is ethyl & in chain-B. it is methyl. Alphabetically ethyl will be preferred. So, chain-A is selected

2. Numbering of the parent carbon chain:

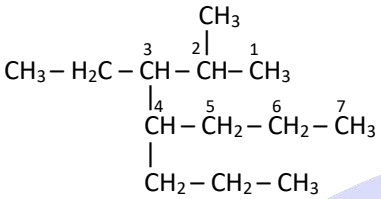
The numbering is done in such a way that the branched carbon atoms get the lowest possible number:

Note: (1) Write the substituents in place of secondary prefix with their appropriate locations in alphabetical order.

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

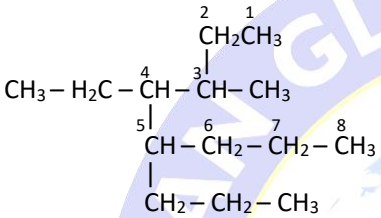
(3) Prefixes di, tri, tetra etc. are not considered in deciding alphabetical order of simple substituents but considered for complex substituents.
(4) Iso & Neo is considered for alphabetical seniority order.
(5) Numbers are separated from each other by commas(,).
(6) Numbers are separated from words by hyphens and there is no break between name of substituents and word root.

Ex. (i)



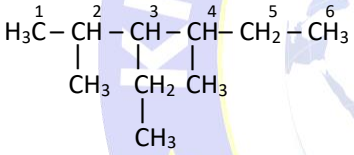
3–Ethyl–2–methyl–4–propylheptane

(ii)



4-Ethyl-3-Methyl-5-propyloctane

(iii)



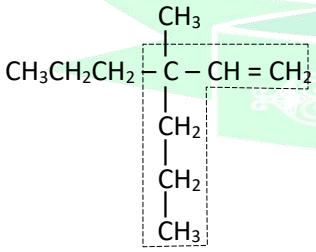
3–Ethyl–2,4–dimethylhexane

IUPAC nomenclature of Alkenes/Alkynes/Alkenyne

1. Alkenes:

Functional group: 

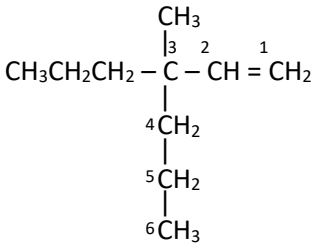
(1) Select the longest carbon chain containing carbon-carbon double bond. This need not be the longest chain in the compounds as whole parent name will be alkene corresponding to number of carbon atoms in the longest chain.

Ex. 

Longest chain has 6 atoms ⇒ parent name = hexene

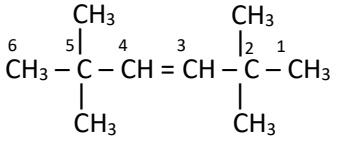
(2) carbon atoms in the longest chain is numbered from that end in such a way that doubly bonded carbon atom gets the lowest number. The position of double bond is indicated by the smaller of the numbers assigned to two carbon atoms of double bond.

The above example can be numbered as,



Position of double bond will be indicated as no. 1, Hence name will be 3–Methyl–3–propylhex–1–ene

Ex.

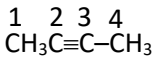


2,2,5,5-Tetramethylhex-3-ene

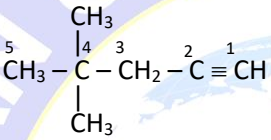
2. Alkynes

Parent chain selection and numbering of longest chain is exactly same as that for alkenes.

Ex.



But-2-yne



4,4–Dimethylpent–1–yne

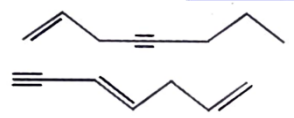
3. Alkenyne (containing both double and triple bonds)

Numbering is done in a manner that double and triple bonds get the lowest possible number. If double bond and triple bond both have same number then double bond is prefer over triple bond.

Ex. **$HC \equiv C - CH_2 - CH = CH_2$**

1 2 3 4 5 (numbering is done from alkyne) ★ **(wrong)**

5 4 3 2 1 (numbering is done from alkene) **(Correct)**



Oct-1-en-4-yne

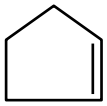
Hepta-3,6-dien-1-yne

SPOT LIGHT

Naming acyclic compounds
Step 1: Determining the primary functional group
Step 2: Determining the primary carbon chain
Step 3: Naming the primary carbon chain
Step 4: Numbering the primary carbon chain
Step 5: Indicating the position of the primary functional group
Step 6: Naming the substituents
Step 7: Assigning configurations
Step 8: Assembling the entire name

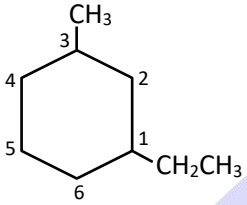
IUPAC nomenclature of alicyclic compounds

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

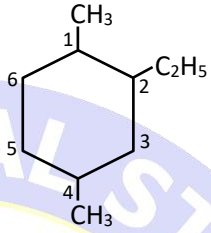
Ex.  

Cyclobutene Cyclopentene

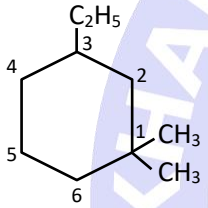
(2) The numbering of the carbon atoms in the ring is done in such a way that the substituent which comes first the alphabetical order is given the lowest possible number but it does not violate the lowest set of locants

Ex. 

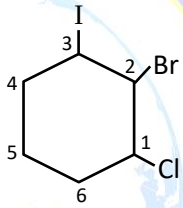
1–Ethyl–3–methyl cyclohexane



2–Ethyl–1,4–dimethyl cyclohexane

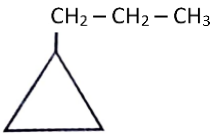


3–Ethyl–1,1–dimethyl cyclohexane



2–Bromo–1–chloro–3–iodocyclohexane

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

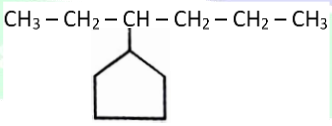
Ex. 

Propylcyclopropane

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

Ex. 

2–Cyclopropylbutane



3–Cyclopentylhexane

(5) (a) If ring has unsaturation and side chain is saturated then ring is selected as parent chain.

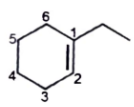
(b) If side chain has unsaturation and ring is saturated then side chain is selected as parent chain.

(c) If both have unsaturation the chain with maximum unsaturation has selected as parent chain.

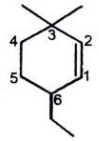
(d) If equal unsaturation then longest chain is select as parent chain.

(e) If unsaturation and number of carbon atoms both are equal then ring is selected as parent chain.

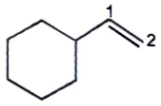
Ex.



1-Ethylcyclohex-1-ene



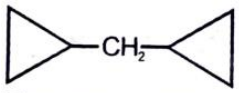
6-Ethyl-3,3-dimethylcyclohex-1-ene



Cyclohexyl ethene

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

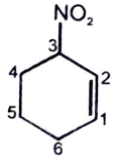
Ex.



Dicyclopropylmethane

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

Ex.



3-Nitrocyclohex-1-ene

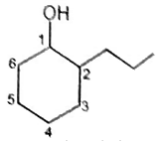
(8) If a compound contains an alicyclic ring directly linked to the benzene ring, It is named as a derivative of benzene.

Ex.

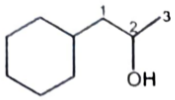
Cyclohexylbenzene

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

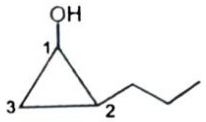
Ex.



2-Propylcyclohexan-1-ol



1-Cyclohexylpropan-2-ol

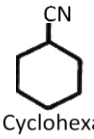


2-Propyl cyclopropan-1-ol

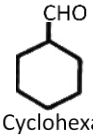
(10) When chain terminating functional group is directly attached with ring then ring is taken as parent chain & special suffix is used for this functional group.

Functional Group	Suffix
CHO	Carbaldehyde
COOH	Carboxylic Acid
COX	Carbonyl halide
COOR	Alkyl Carboxylate
$CONH_2$	Carboxamide
CN	Carbonitrile

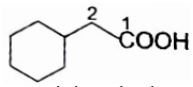
Ex.



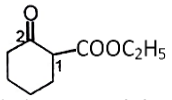
Cyclohexanecarbonitrile



Cyclohexanecarbaldehyde



2-Cyclohexyl ethanoic acid



Ethyl 2-oxocyclohexane-1-carboxylate

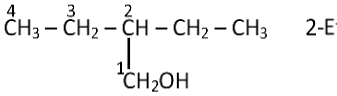
SPOT LIGHT

Naming cyclic compounds
Step 1: Determining the primary functional group
Step 2: Determining the primary carbon chain
Step 3: Naming the primary carbon chain
Step 4: Numbering the primary carbon chain
Step 5: Indicating the position of the primary functional group
Step 6: Naming the substituents
Step 7: Assigning configurations
Step 8: Assembling the entire name

IUPAC nomenclature of compounds containing functional groups

1. Rules for non chain terminating functional groups

(1) Parent chain: Select the longest possible chain with maximum functional group and maximum unsaturation without caring whether it also denotes the longest possible chain or not.

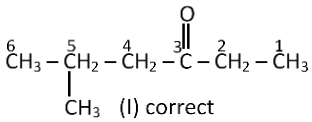
Ex. 

2-Ethyl butan-1-ol

(Parent chain contains four rather than five carbon atoms)

(2) Lowest number for the functional group

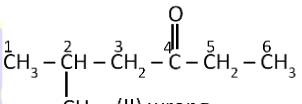
Numbering is done from that side of the chain which gives lowest locant to the principal group followed by double and triple bonds.

Ex. 

(I) correct

5-Methyl hexane-3-one

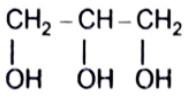
(>C = O group gets lowest number 3)



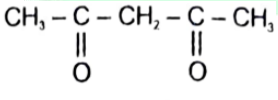
(II) wrong

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

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

Ex. 

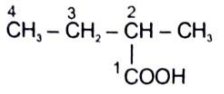
Propane – 1,2,3 – triol

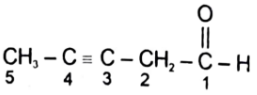


Pentane-2, 4-dione

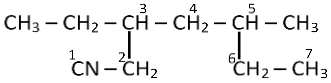
2. Rules for chain terminating functional groups

(1) When a chain terminating functional group such as **– CHO, – COOH, – COOR, –CONH$_2$, –COCl, –C≡N** etc. is present, it is always given number 1 (one.)

Ex. 
2-Methylbutan-1-oic acid

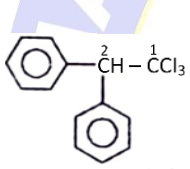

Pent-3-yn-1-al

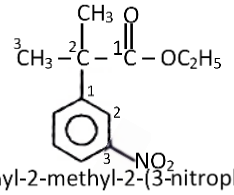
Example: Write the IUPAC name of



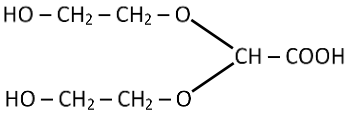
Solution:
1. The longest chain containing functional group is of 7 carbon atoms. Therefore, the word root is hept and the chain is numbered as shown.
2. There is no multiple bond in it. Hence, the primary suffix is ane.
3. The functional groups is –CN. Hence, secondary suffix is nitrile
4. Moreover,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

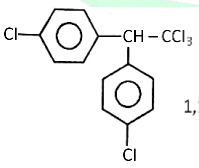
(2) The name for benzene as substituent is phenyl. In case the phenyl ring is further substituted, the carbon atoms of the ring directly attached to the parent chain is such a ways that the substituent on the gets the least possible number. For example


1,1,1-Trichloro-2,2-diphenylethane


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

(3) If the organic molecule contains more than one similar complex substituents, then the numeral prefixes such as di, tri, tetra etc. are replaced by bis, tris, tetrakis etc. respectively.

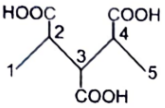
Ex. 
2, 2-Bis(2-hydroxyethoxy) ethanoic acid

Ex.  (IUPAC NAME)

1,1,1-Trichloro-2,2-bis(4-chlorophenyl) ethane

Common name is D.D.T. (dichloro diphenyl trichloro ethane) & is used as insecticide.

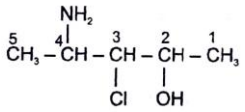
(4) When 3 or more principal functional group are directly attached with an open chain, then special suffix used.

Ex. 
Pentane-2,3,4-tricarboxylic acid

3. Rules for IUPAC nomenclature of polyfunctional compounds:

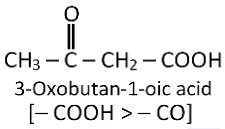
(1) When an organic compound contains two or more different functional groups then senior functional group is selected as the principal functional group while other functional groups are treated as substituents.

(2) Some functional group such as all halo groups (fluoro, bromo, chloro, iodo), nitroso (NO) nitro ($-NO_2$) and alkoxy (–OR) are always treated as substituent groups.

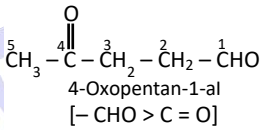
Ex. 

4-Amino-3-chloropentan-2-ol
(– NH_2 & – Cl group treated as substituent)

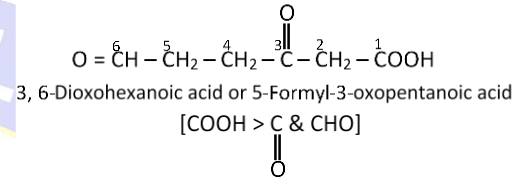
Numbering the principle chain order is
[Principal functional group > double bond > triple bond > substituents]

Ex. 

3-Oxobutan-1-oic acid
[– COOH > – CO]

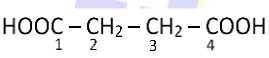


4-Oxopentan-1-al
[– CHO > C = O]

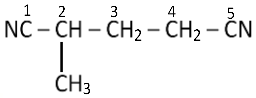


3, 6-Dioxohexanoic acid or 5-Formyl-3-oxopentanoic acid
[COOH > C & CHO]

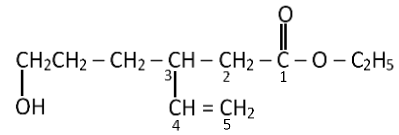
(3) If more than one same chain terminating group are present then the principal chain is selected including the functional groups and numbering is done from that side which gives lowest locant to unsaturation and substituents.

Ex. (a) 

Butane-1, 4-dioic acid

(b) 

2-Methylpentane 1, 5 dinitrile

(c) 

Ethyl-3-(3-hydoxy propyl) pent-4-enoate

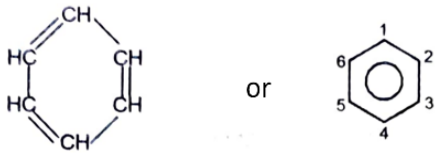
Parent chain contains five rather than six carbon atoms.

Priority List of Functional Groups

-COOH > $-SO_3H$ > -COOR > -COCl > $-CONH_2$ > -CN > HC=O > -CO > -OH > $-NH_2$ > C=C > C-C.

Nomenclature of aromatic compounds

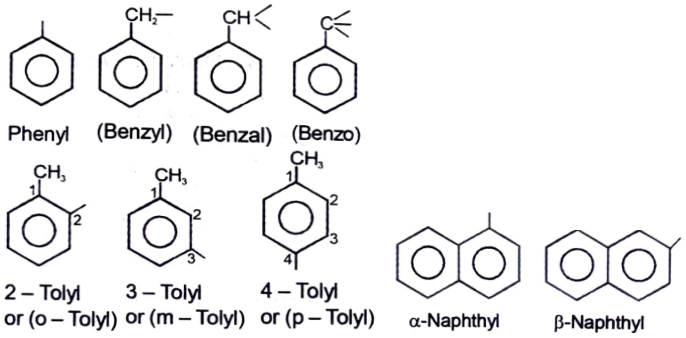
The aromatic compounds are cyclic compounds which contain one or more benzene type rings. Benzene is the simplest hydrocarbon of aromatic series which has planar cyclic ring of six carbon atoms having three double bonds in alternate positions as shown below.



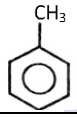
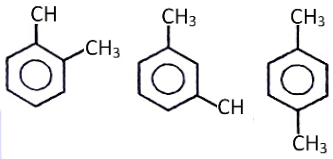
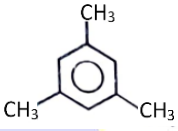
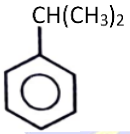
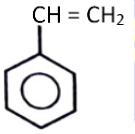
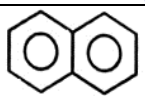
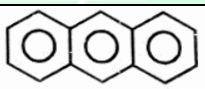
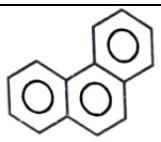
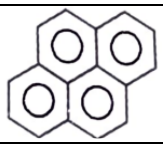
(i) Nuclear substituted : The functional group is directly attached to the benzene ring, in the IUPAC system they are named as derivatives of benzene. The position of the substituents in disubstituted benzenes are indicated either by prefixes such as **o-(ortho) for 1,2**, **m-(meta) for 1, 3** and **p-(para)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

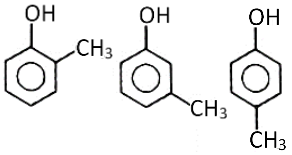
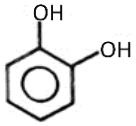
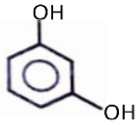
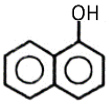
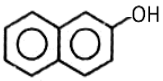
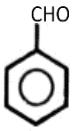
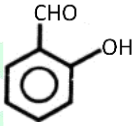
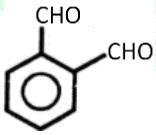
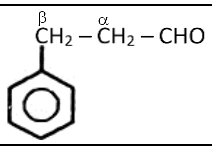
(ii) Side chain substituted : If functional group is present in the side chain of the benzene ring in the IUPAC system, these are usually named as phenyl derivatives of the corresponding aliphatic compounds. The IUPAC and common names of a few important members of each family are given below.

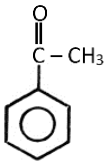
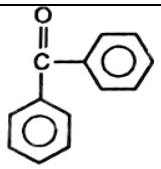
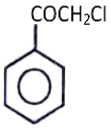
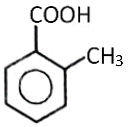
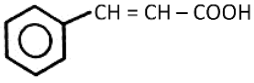
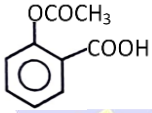
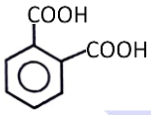
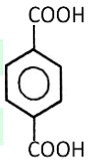
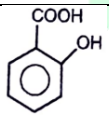
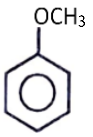
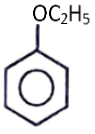
1. Aryl groups :

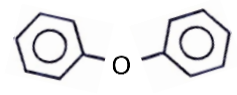
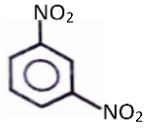
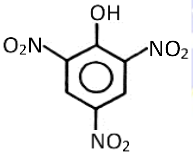
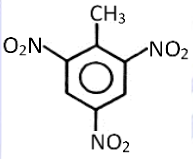
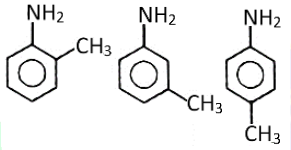
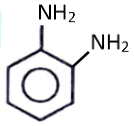
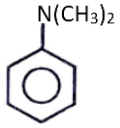


2. Other aromatic examples

S. No.	Compounds	Common Name	IUPAC Name
	Aromatic Hydrocarbons:		
1.		Toluene	Methylbenzene or Toluene
2.		o–Xylene m–Xylene p–Xylene	o– Dimethylbenzene m– Dimethylbenzene p– Dimethylbenzene
3.		Mesitylene	1,3,5 – Trimethyl benzene
4.		Cumene	Iso propyl benzene
5.		Styrene	Phenyl ethene or Ethenylbenzene
6.		Naphthalene	Naphthalene
7.		Anthracene	Anthracene
8.		Phenanthrene	Phenanthrene
9.		Pyrene	Pyrene
	Aromatic Alcohols :		

10.		Carbolic acid	Phenol
11.		o– cresol m– cresol p– cresol	Methyl phenol
12.		Catechol	Benzene-1, 2-diol
13.		Resorcinol	Benzene-1, 3-diol
14.		Hydroquinol	Benzene-1, 4-diol
15.		α-Naphthol	Naphthalen-1-ol
16.		β-Naphthol	Naphthalen-2-ol
	Aromatic Aldehydes :		
17.		Oil of bitter almonds	Benzaldehyde
18.		Salicylaldehyde	2-Hydroxy benzaldehyde (2-Hydroxybenzene carbaldehyde)
19.		Phthalaldeyde	Benzene-1, 2-dicarbaldehyde
20.		β-phenylpropionaldehyde	3-Phenylpropanal
	Aromatic Ketones :		

21.		Acetophenone	Acetophenone
22.		Benzophenone	Benzophenone (Diphenylketone)
23.		Phenacyl chloride	Chloroacetophenone
	Aromatic Acid :		
24.		Benzoic acid	Benzenecarboxylic acid (Benzoic acid)
25.		o-toluic acid	2-Methylbenzene carboxylic acid
26.		Cinnamic acid	3-Phenylprop-2-enoic acid
27.		Aspirin (Acetyl salicylic acid)	2-Ethanoyloxybenzene carboxylic acid
28.		Phthalic acid	Benzene 1, 2,-dicarboxylic acid
29.		Terephthalic acid	Benzene 1, 4-dicarboxylic acid
30.		Salicylic acid	2-Hydroxybenzene carboxylic acid
	Aromatic Ethers :		
31.		Anisole	Methoxybenzene
32.		Phenetol	Ethoxybenzene

33.		Diphenyl ether	Phenoxybenzene
	Aromatic Nitro Compound :		
34.		Oil of mirbane	Nitrobenzene
35.		–	1, 3-Dinitrobenzene (m-Dinitrobenzene)
36.		Picric acid	2, 4, 6-Trinitrophenol
37.		–	2, 4, 6-Trinitrotoluene(TNT) an explosive
	Aromatic Amines :		
38.		Aniline	Aniline (Benzenamine)
39.		o– Toluidine m– Toluidine p– Toluidine	Methylaniline
40.		o-Phenylenediamine	Benzene-1,2-diamine
41.		N,N-Dimethylaniline	N,N-Dimethylbenzenamine

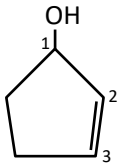
Some important 1993 recommendations for IUPAC nomenclature of organic compounds:

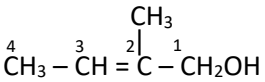
1. Locants (numerals / letters) are placed immediately before the part of the name to which they relation for example:

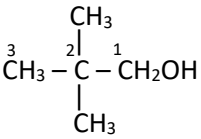
   $CH_3CH_2CH = CH_2$ should be named as but-1-ene

   $CH_3CH_2CH_2OH$ should be named as propan-1-oI

Similarly, a few more examples are given as following:

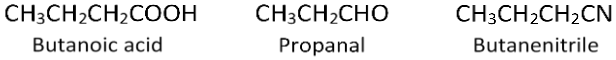






Cyclopent-2-en-1-ol 2-Methylbut-2-en-1-ol 2,2-Dimethylpropan-1-ol

2. The locant 1 is often omitted when there is no ambiguity(open to interpretation). For example.



Butanoic acid Propanal Butanenitrile

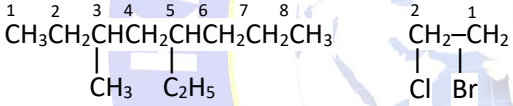
In all the above examples locant 1 for the functional group is omitted because the position of the functional group is unambiguous. However, in the following cases the position of the functional group must be mentioned.

Propan-1-ol Propan-1-amine

Here, we cannot write simply propanol (or propanamine) because there are two propanols – propan-1-ol and propan-2-ol.

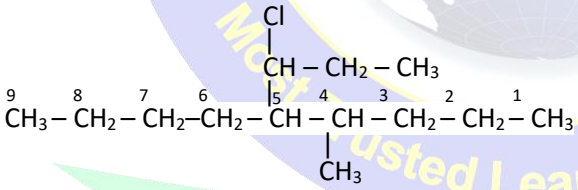
3. Arrangement of Prefixes

(i) Simple prefixes such as methyl, ethyl, chloro, nitro, hydroxy, etc. are arranged alphabetically. The prefixed di, tri, etc. are however not considered for comparison.

Ex. 

5-Ethyl-3-methyl octane 1-Bromo-2-chloroethane

(ii) The name of a prefix for a substituted substituent is considered to begin with the first letter of its completely name.

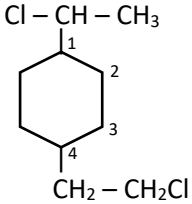
Ex. 

5-(1-Chloropropyl)-4-methylnonane

From the substituted 1-chloropropyl, 'C' is taken as the first letter.

(iii) When two or more prefixes consist of identical roman letters priority for citation is given to the group which has lower numbered similar substituent in the group.

For example,



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

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

QUICK FOLLOW UP

Degree of unsaturation: Deficiency of 2H atoms with respect to fully saturated acyclic hydrocarbon is equivalent to One DU. It is also known as Hydrogen Deficiency Index (HDI) or Double Bond Equivalence (DBE)

Types of Organic formula

Molecular formula

The molecular formula of an organic compound simply shows the number of each type of atom present. It tells you nothing about the bonding within the compound.

$C_4H_8O_2$

Empirical formula

The empirical formula of an organic compound gives the simplest possible whole number ratio of the different types of atom within the compound.

C_2H_4O

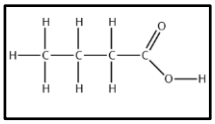
Condensed formula

The condensed formula is also text based; here, each carbon atom is listed separately, with atoms attached to it following. An exception is cyclic parts of molecules, e.g. benzene, where the carbons are grouped.

$CH_3CH_2CH_2COOH$

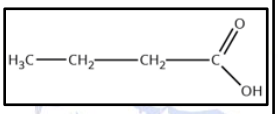
Displayed formula

A displayed formula shows all of the atoms and all of the bonds present in an organic compound. The bonds are represented as lines.



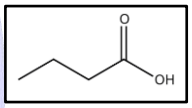
Structural formula

Similar to displayed formula-not all bonds are shown, although all atoms are still indicated using subscript numbers. Carbon hydrogen bonds are often simplified.



Skeletal formula

In a skeletal formula, most hydrogen atoms are omitted, and line ends or vertices represent carbons. Functional groups and atoms other than carbon or hydrogen are still shown. Easiest to drown & commonly used.



Name of an Organic Compound is made of

Prefix	+	Root	+	Primary Suffix	+	Secondary suffix
Substituent		Number of carbons in longest chain		Types of chain		If functional group is present
3-methyl		pent		an–		2-one

Basic Steps to Name an Organic Compound

1. Find the longest carbon chain which contains functional group
2. Number the carbon atoms present in the parent chain
3. Find the word root
4. Look for the branch attached to the parent chain
5. Write the prefix + word root + suffix and complete the name