IUPAC NOMENCLATURE & STRUCTURAL ISOMERISM

1. SECTION (A) : FUNDAMENTAL OF ORGANIC CHEMISTRY

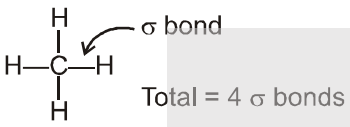
Th1:

1.1 Bonding in organic compounds :

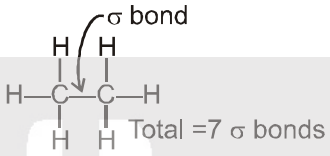
Two types of covalent bond exist in organic compounds.

(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



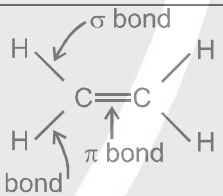
In C_2H_6 molecule



(b) Multiple bond (π) :

Any other bond with σ bond is π bond.

Ex.

(i) In ethane Molecule		(ii) In ethyne molecule	
	Total σ = 5		Total σ = 3
	π = 1		π = 2

Que. Calculate σ and π bond in following compounds.

(a) $HC \equiv CCH=CHCH_3$

(b) $CH_2 = C = CHCH_3$

Sol.

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

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

1.2 Some important definitions :

D1:

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

D2:

(ii) **Homologous series:** Homologous series may be defined as a series of similarly 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.

Th2:

1.3 Structural representation of organic compounds :

There are three ways for representation of organic compounds :

(i) Complete structural formula:

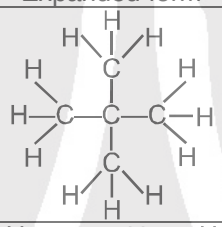
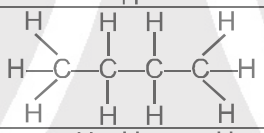
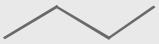
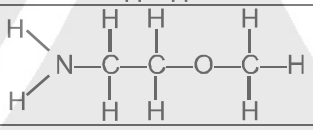
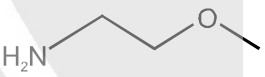
Such a structural formula focuses on the electrons involved in bond formation. A single dash (–) represents a single bond, double dash (=) is used for double bond and a triple dash (≡) represents triple bond. Lone- pairs of electrons on heteroatoms (e.g., oxygen, nitrogen, sulphur, halogens etc.) may 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 compound is called a condensed structural formula.

(iii) Bond line formula:

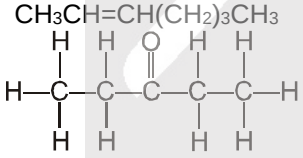
In this formula, carbon and hydrogen atoms are not shown and the lines representing carbon-carbon bonds are drawn in a zig-zag fashion. The only atoms specifically written are oxygen, chlorine, nitrogen etc.

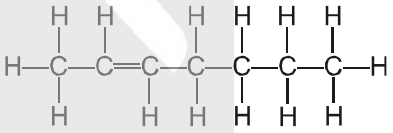
Condensed form	Expanded form	Bond line form
$C(CH_3)_4$		
$CH_3(CH_2)_2CH_3$		
$H_2N(CH_2)_2OCH_3$		

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

(a) $CH_3CH_2COCH_2CH_3$

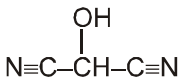
(b) $CH_3CH{=}CH(CH_2)_3CH_3$

Sol. **(a)** 

(b) 

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

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

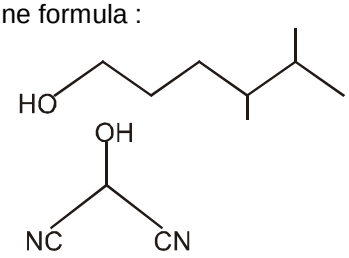
(b) 

Sol. Condensed formula :

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

(b) $HOCH(CN)_2$

Bond-line formula :



Th3:

1.4 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 rings and also helpful in determining the structure of the molecule.

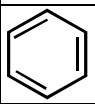
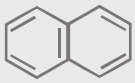
D3: **Definition:** Deficiency of 2H atoms with respect to fully saturated acyclic hydrocarbon is equivalent to One DU. It is also known as Hydrogen Deficiency Index (HDI) or Double Bond Equivalence (DBE)

$H_3C-H_2C-CH_3$ (DU = 0) $\xrightarrow{-2H}$ [$CH_3-CH=CH_2$ or  (DU = 1)] $\xrightarrow{-2H}$ $CH_3-C\equiv CH$ or $CH_2=C=CH_2$ or  (DU = 2)

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

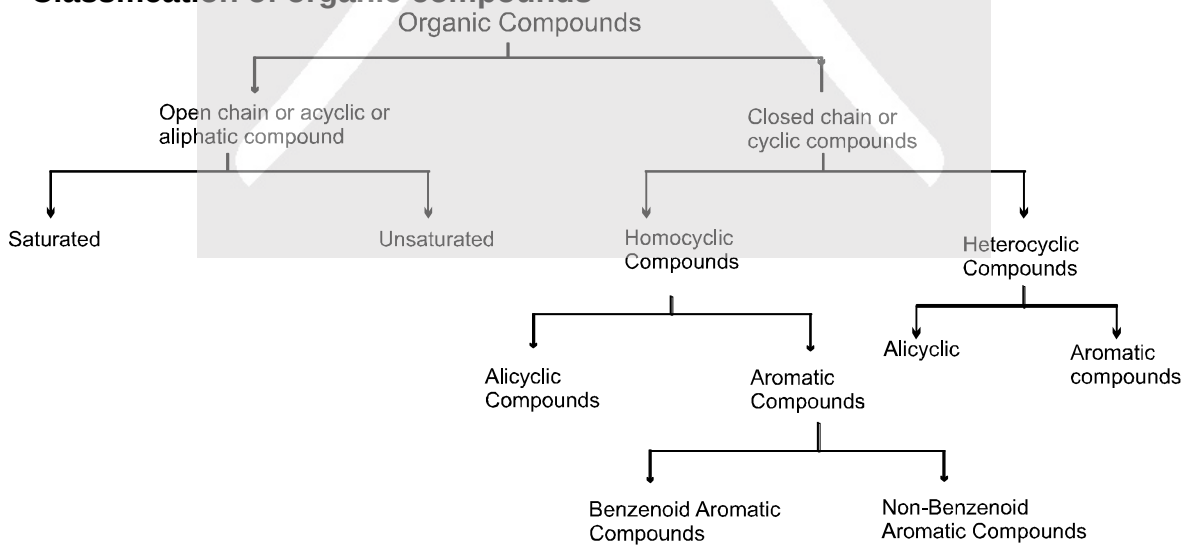
Where n = number of carbon atoms in the molecule

Note : Total no. of cyclic rings + double bonds will gives us degree of unsaturation.
One double bond = one DU
One ring = one DU
One triple bond = two DU

Ex.	**(i)**	$CH_2=CH_2$	DU = $\frac{(2\times2+2)-4}{2}$ = 2/2 = 1	**(ii)**		DU = 2
	(iii)		DU = 4	**(iv)**		DU = 7

Th4:

1.5 Classification of organic compounds



Th5:

1.6 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 based on their structural features. This has given organic chemistry a logical and systematic shape. Examples are as follows :

1.6.1 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

1.6.2 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.

$CH_2=CH_2$	$CH_3–CH=CH_2$	$CH_3–CH_2–CH=CH_2$	$CH_3-\underset{\displaystyle CH_3}{\overset{|}{C}}=CH_2$
ethylene	propylene	butylene	Isobutylene

1.6.3 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
$CH_3–CH_2–C\equiv CH$	–	Ethylacetylene
$CH_3–C\equiv C–CH(CH_3)_2$	–	Methyl isopropyl acetylene

1.6.4 Some names of hydrocarbon groups

(A) Alkyl, Alkenyl & Alkynyl groups

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

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

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

Ex.

$\text{methane} \xrightarrow[+yl]{-ane} \text{methyl} \quad \left(CH_4 \xrightarrow{-H} -CH_3\right)$

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

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

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

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

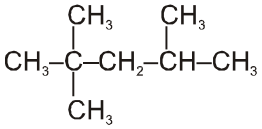
remove H from C_2 → $CH_2 = \underset{\displaystyle CH_3}{\overset{|}{C}} -$ Isopropenyl group

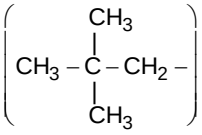
$HC\equiv CH \xrightarrow{-H} HC\equiv C-$ (Ethynyl) ; $H_3C–C\equiv CH \xrightarrow{-H} H_3C–C\equiv C-$ (propynyl)

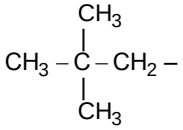
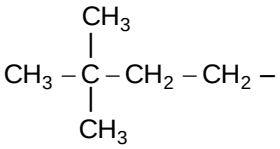
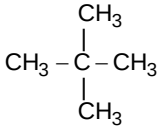
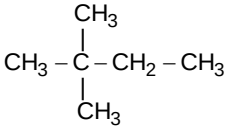
(B) Iso alkyl group : A compound having $-\underset{\displaystyle CH_3}{\overset{|}{CH}}-CH_3$ group is called iso alkyl group.

Ex.

$CH_3-\underset{\displaystyle CH_3}{\overset{|}{CH}}-$	$CH_3-\underset{\displaystyle CH_3}{\overset{|}{CH}}-CH_2-$	$CH_3-\underset{\displaystyle CH_3}{\overset{|}{CH}}-CH_2-CH_2-$	$CH_3-\underset{\displaystyle CH_3}{\overset{|}{CH}}-CH_2-CH_3$
Iso propyl	Iso butyl	isopentyl	Iso pentane

Exception : Isooctane 

(C) Neo alkyl group : Compound having  group is called neo alkyl group.

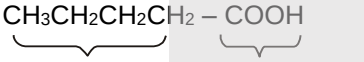
Ex.    

Neopentyl Neohexyl Neopentane Neohexane

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

Ex. 

Residue Functional Group

2. SECTION (B) : IUPAC-NOMENCLATURE OF ALKANE & CYCLOALKANE

Th6:

2.1 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

2.2 Word root :

It is the basic unit of the name. It denotes the number of carbon atoms present in the principal 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	Hexadeca	100	Cent & Hect

2.3 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

2.4 Secondary suffix :

A secondary suffix is then 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.

	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 – C(=O) – O – C(=O) – R	Alkanonic Anhydride	– oic anhydride (carboxylic anhydride)	----------
4.	R – COOR	Alkyl alkanoate	– oate (carboxylate)	alkoxy carbonyl or alkanoyl oxy
5.	R – C(=O) – X	Alkanoyl halide	–oyl halide (carbonyl halide)	halo carbonyl
6.	R – C(=O) – NH_2	Alkanamide	– amide (carboxamide)	carbamoyl
7.	R – C ≡ N	Alkanenitrile	– nitrile (carbonitrile)	cyano
8.	R – C(=O) – H	Alkanal	– al (carbaldehyde)	formyl / oxo
9.	R – C(=O) – R	Alkanone	– one	oxo
10.	R – OH	Alkanol	– ol	hydroxy
11.	R – SH	Alkanethiol	– thiol	mercapto
12.	R – NH_2	Alkanamine	– amine	amino

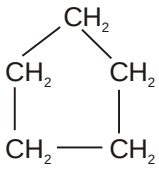
The following examples illustrate the use of word root, primary suffix and secondary suffix in naming of organic compounds.

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	Propanenitrile
CH_2=CHCHO	Prop	en(e)	al	Propenal
HC ≡ CCOOH	Prop	yn(e)	oic acid	Propynoic acid

2.5 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 simply indicates that the compound is acyclic or open chain.

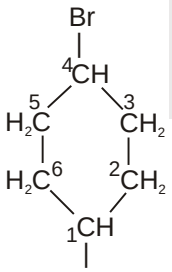
2.6 Secondary prefix :

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

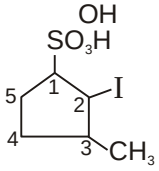
Example :

Organic compounds	Secondary prefix	Word root	Primary suffix	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. 

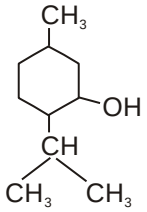
4-Bromo + cyclo + hex + an (e) + 1-ol

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

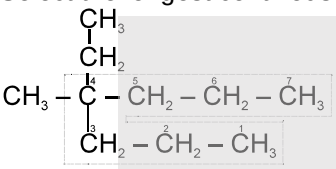
Here	Secondary prefix	=	2-Isopropyl-5-methyl
	Primary prefix	=	cyclo
	Word root	=	hex
	Primary suffix	=	an(e)
	Secondary suffix	=	ol

Th7:

3. IUPAC NOMENCLATURE OF BRANCHED / COMPLEX ALKANES

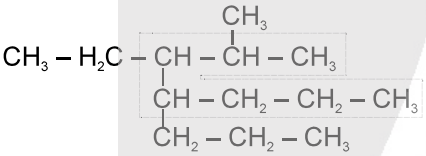
3.1 Parent carbon chain selection :

(a) Select the longest continous carbon chain in the molecule.



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

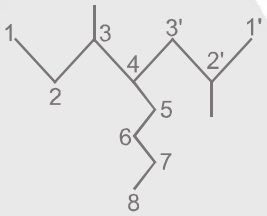
(b) When chains of equal lengths are competing for selection then that chain is selected which has more number of substituents/branches.



longest chain has 7 carbon & 3 substituents

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

Ex. Here, 2 choices for longest chain

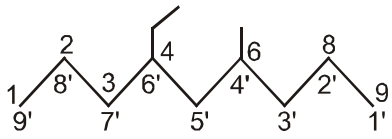


Chain- (A) 1–2–3–4–5–6–7–8 Chain- (B) 1'–2'–3'–4–5–6–7–8

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.

3.2 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.

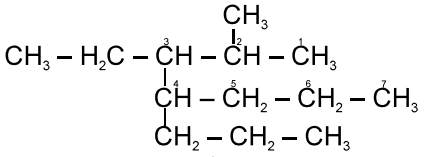
(3) Prefixes di, tri, tetra etc. are not considered in deciding alphabetical order for simple substituents but considered for complex substituents.

(4) Iso & Neo is considered for alphabetical seniority order.

(5) Numbers are separated from each other by commas(,).

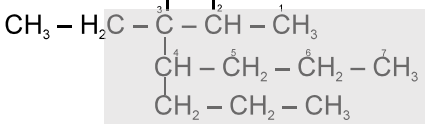
(6) Numbers are separated from words by hyphens and there is no break between name of substituents and word root.

Ex. **(i)**



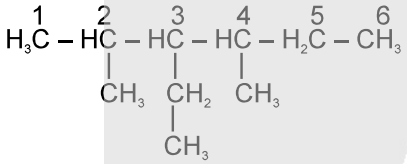
3-Ethyl-2-methyl-4-propylheptane

(ii)



3-Ethyl-2,3-dimethyl-4-propylheptane

(iii)



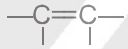
3-Ethyl-2,4-dimethylhexane

4. SECTION (C) : IUPAC-NOMENCLATURE OF ALKENE, CYCLOALKENE, POLYENES & ALKYNE

Th8:

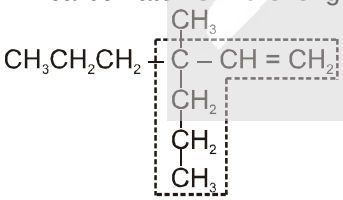
4.1 IUPAC nomenclature of Alkenes/Alkynes/Alkenyne

4.1.1 Alkenes :

Functional group : 

(1) Select the longest carbon chain containing carbon–carbon double bond. This need not be the longest chain in the compound as a whole. Parent name will be alkene corresponding to number of carbon atoms in the longest chain.

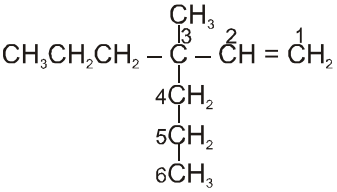
Ex.



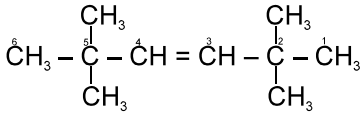
Longest chain has 6 atoms ⇒ parent name = hexane

(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,

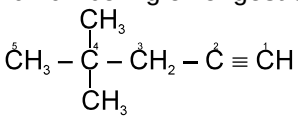


Position of double bond will be indicated as no. 1, Hence name will be 3-Methyl-3-propylhex-1-ene

Ex.  , 2,2,5,5-Tetramethylhex-3-ene

4.1.2 Alkynes

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

Ex. $CH_3C{\equiv}C{-}CH_3$ But-2-yne  4,4-Dimethylpent-1-yne

4.1.3 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.

$HC \equiv C - CH_2 - CH = CH_2$

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

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

Ex.

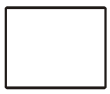
(a)  Oct-1-en-4-yne

(b)  Hepta-3,6-dien-1-yne

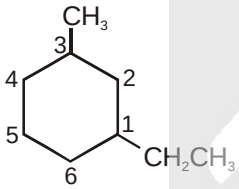
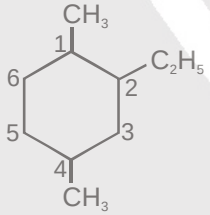
Th9:

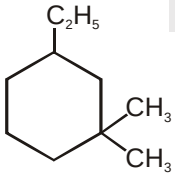
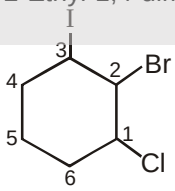
5. IUPAC NOMENCLATURE OF ALICYCLIC COMPOUNDS

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

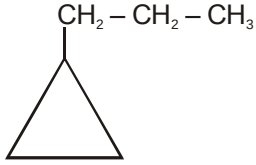
Ex.  Cyclobutane  Cyclopentene

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

Ex.  1-Ethyl-3-methyl cyclohexane  2-Ethyl-1,4-dimethyl cyclohexane

 3-Ethyl-1,1-dimethyl cyclohexane  2-Bromo-1-chloro-3-iodocyclohexane

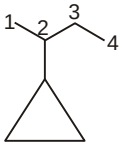
(3) When the ring contains more or equal number of carbon atoms than the alkyl group attached to it, then it is named as a derivative of cycloalkane and the alkyl group is treated as substituent

Ex. 

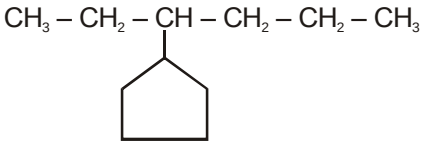
Propylcyclopropane

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

Ex.



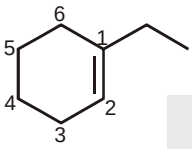
2-Cyclopropylbutane



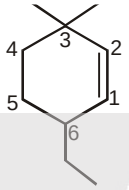
3-Cyclopentylhexane

(5) If ring has unsaturation and side chain is saturated then ring is selected as parent chain.
If side chain has unsaturation and ring is saturated then side chain is selected as parent chain.
If both have unsaturation the chain with maximum unsaturation has selected as parent chain.
If equal unsaturation then longest chain is selected as parent chain.
If unsaturation and number of carbon atoms both are equal then ring is selected as parent chain.

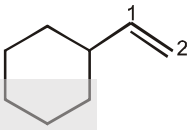
Ex.



1-Ethylcyclohex-1-ene



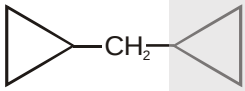
6-Ethyl-3,3-dimethylcyclohex-1-ene



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.

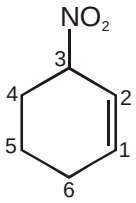
Ex.



Dicyclopropylmethane

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

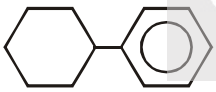
Ex.



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.

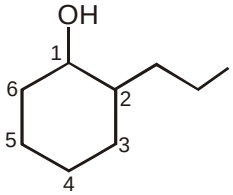
Ex.



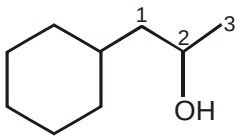
Cyclohexylbenzene

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

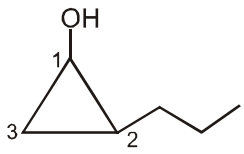
Ex.



2-Propylcyclohexan-1-ol



1-Cyclohexylpropan-2-ol

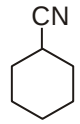


2-Propyl cyclopropan-1-ol

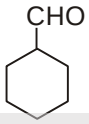
(10) When chain terminating functional group is directly attached with ring then ring is taken as parent chain & special suffix is used for this functional group.

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

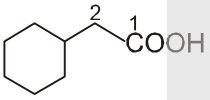
Ex.



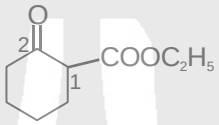
Cyclohexanecarbonitrile



Cyclohexanecarbaldehyde



2-Cyclohexyl ethanoic acid



Ethyl 2-oxocyclohexane-1-carboxylate

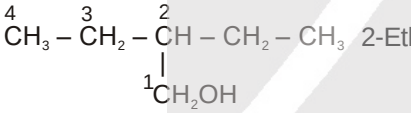
6. SECTION (D) : IUPAC NOMENCLATURE OF NON-CHAIN TERMINATING FUNCTIONAL GROUPS

Th10:

6.1 IUPAC nomenclature of compounds containing functional groups

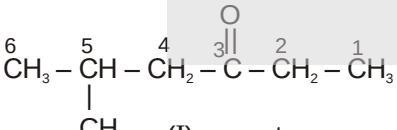
6.1.1 Rules for non chain terminating functional groups

(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 principle functional group followed by double and triple bonds.

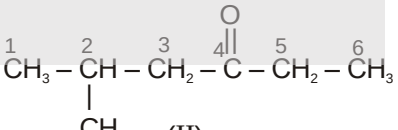
Ex.



(I) correct

5-Methyl hexan-3-one

($>C=O$ group gets lowest number 3)

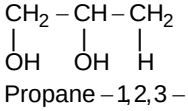


(II) wrong

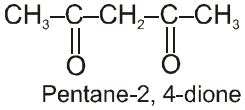
($>C=O$ group gets number 4 which is not lowest)

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

Ex.



Propane – 1,2,3 – triol

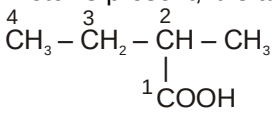


Pentane-2, 4-dione

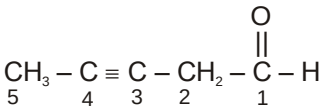
7. SECTION (E) : IUPAC NOMENCLATURE OF CHAIN TERMINATING FUNCTIONAL GROUPS

7.1 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.)



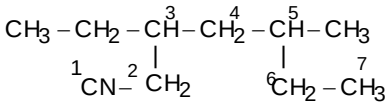
2-Methylbutan-1-oic acid



Pent-3-yn-1-al

Ex.

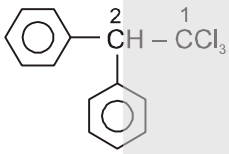
Que. Write the IUPAC name of



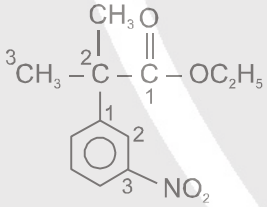
Sol.

1. The longest chain containing functional group is of **7** carbon atoms. Therefore, the word root is hept & 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 substitued, the carbon atoms of the ring directly attached to the parent chain in such a ways that the substituent on the ring gets the least possible number. For example



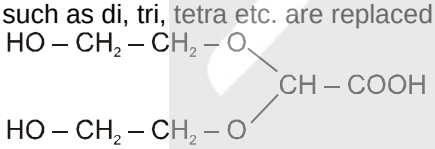
1,1,1-Trichloro-2,2-diphenylethane



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

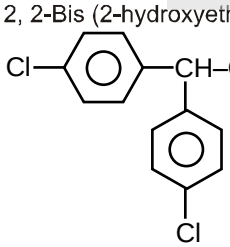
(3) If the organic molecule contains more than one similar complex substitutents, then the numeral prefixes such as di, tri, tetra etc. are replaced by bis, tris, tetrakis etc. respectively.

Ex.



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

Ex.

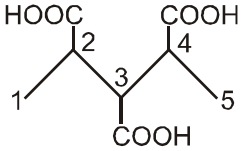


IUPAC Name : 1,1,1-Trichloro-2,2-bis(4-chlorophenyl)ethane

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

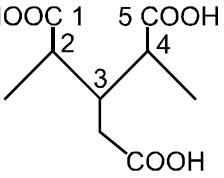
(4) When 3 or more principle functional groups are directly attached with an open chain, then special suffix is used.

Ex.



Pentane- 2,3,4–tricarboxylic acid.

Not true for



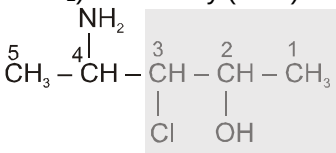
3-Carboxymethyl-2,4- dimethylpentanedioic acid

7.2 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.



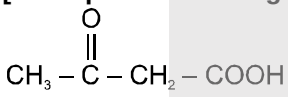
4-Amino-3-chloropentan-2-ol

(– NH_2 & – Cl group treated as substituent)

Numbering the principal chain order is

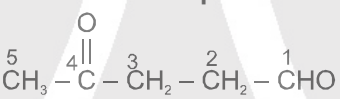
[Principal functional group > double bond > triple bond > substituents]

Ex.



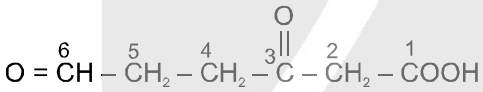
3-Oxobutan-1-oic acid

[– COOH > – CO]



4-Oxopentan-1-al

[– CHO > C=O]



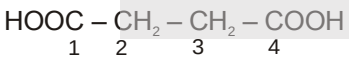
3, 6-Dioxohexanoic acid or 5-Formyl-3-oxopentanoic acid

[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 numbring is done from that side which gives lowest locant to unsaturation and substituents.

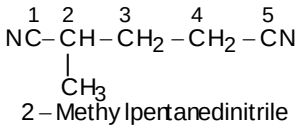
Ex.

(a)



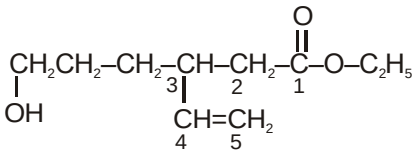
Butane-1, 4-dioic acid

(b)



2 – Methylpentanedinitrile

(c)



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

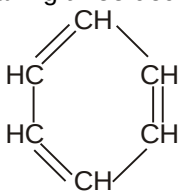
Parent chain contains five rather than six carbon atoms.

8. SECTION (F) : IUPAC-NOMENCLATURE OF AROMATIC COMPOUNDS

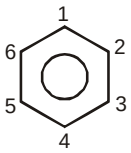
Th11:

8.1 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.



or

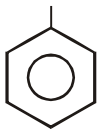


(i) Nuclear substituted: The functional group is directly attached to the benzene ring, in the IUPAC system they are named as derivatives of benzene. The position of the substituents in disubstituted benzenes are indicated either by prefixes such as o-(ortho) for 1,2,m-(meta) for 1, 3 and p-(para) for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

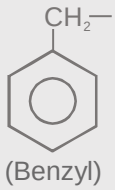
(ii) Side chain substituted: If functional group is present in the side chain of the benzene ring in the IUPAC system, these are usually named as phenyl derivatives of the corresponding aliphatic compounds.

The IUPAC and common names of a few important members of each family are given below.

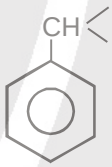
1. Aryl groups :



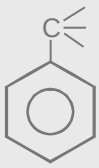
Phenyl



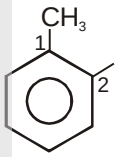
(Benzyl)



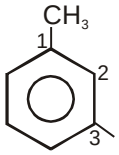
(Benzal)



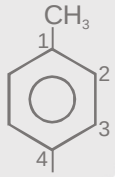
(Benzo)



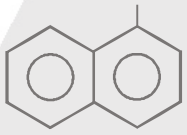
2 – Tolyl or (o – Tolyl)



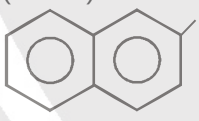
3 – Tolyl
or (m – Tolyl)



4 – Tolyl
or (p – Tolyl)

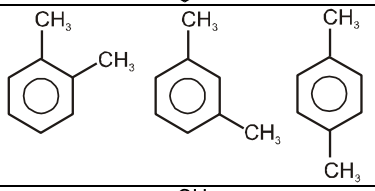
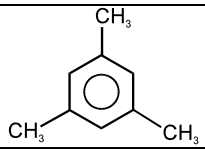


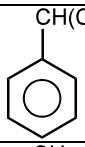
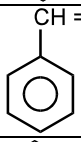
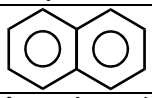
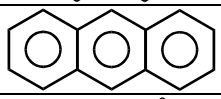
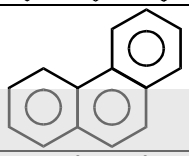
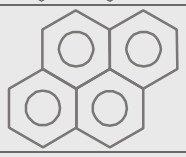
α-Naphthyl



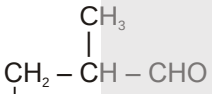
β-Naphthyl

8.2 Other aromatic examples

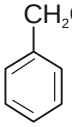
S.No.	Compounds	Common Name	IUPAC Name
	Aromatic Hydrocarbons		
1		Toluene	Methylbenzene or Toluene
2		Xylene (o,m,p)	(o,m,p) Dimethylbenzene
3		Mesitylene	1,3,5-Trimethylbenzene

4		Cumene	Isopropylbenzene
5		Styrene	Phenyl ethane or Ethenylbenzene
6		Naphthalene	Naphthalene
7		Anthracene	Anthracene
8		Phenanthrene	Phenanthrene
9		Pyrene	Pyrene

Que. Write IUPAC name of following aromatic compounds



(a) 

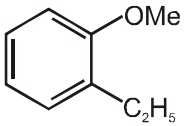
(b) 

Ans.

(a) 2-Methyl-3-phenylpropanal
(b) Methoxyphenylmethane (Benzyl methyl ether)

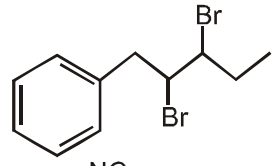
Que. Write the structural formula of :
(a) o-Ethylanisole,
(b) p-Nitroaniline,
(c) 2,3-Dibromo-1-phenylpentane
(d) 4-Ethyl-1-fluoro-2-nitrobenzene.

Ans.

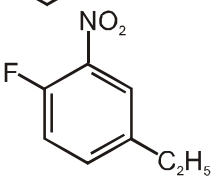
(a) 

(b) 

(c)



(d)

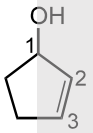


Th12:

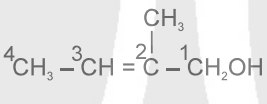
9. SOME IMPORTANT 1993 RECOMMENDATIONS FOR IUPAC NOMENCLATURE OF ORGANIC COMPOUNDS :

1. Locants (numerals and / or letters) are placed immediately before the part of the name to which they relate. For example :

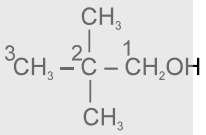
$CH_3CH_2CH = CH_2$ should be named as but-1-ene ; $CH_3CH_2CH_2OH$ should be named as propan-1-ol similarly, a few more examples are given as following :



Cyclopent-2-en-1-ol



2-Methylbut-2-en-1-ol

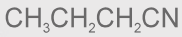


2,2-Dimethylpropan-1-ol

2. The locant 1 is often omitted when there is no ambiguity. For example.

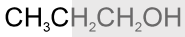
Butanoic acid

Propanal

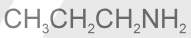


Butanenitrile

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



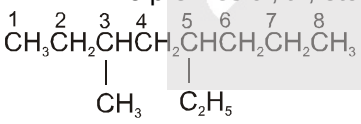
Propan-1-amine

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

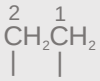
3. Arrangement of Prefixes

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

Ex.



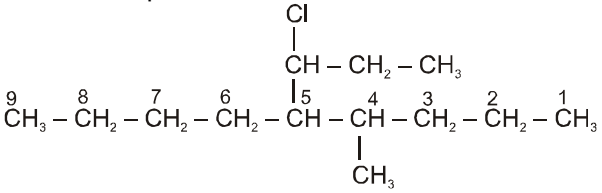
5-Ethyl-3-methyl octane



1-Bromo-2-chloroethane

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

Ex.

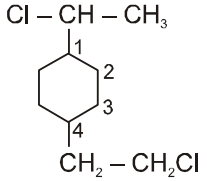


5-(1-Chloropropyl)-4-methyloctane

for 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 contains the lowest locant at the first point of difference.

For example,



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

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

Structural Isomerism

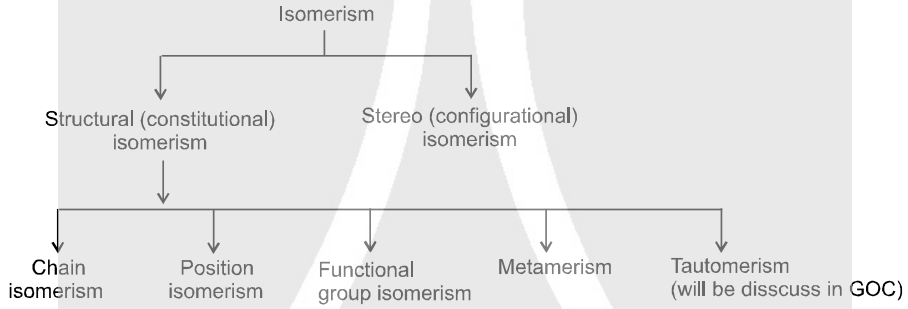
10. SECTION (G) : STRUCTURAL ISOMERISM

D4: Isomerism :

The phenomenon of existence of 2 or more compounds possessing the same molecular formula but different properties is known as isomerism. Such compounds are known as isomers.

Th13:

10.1 Classification of isomerism



10.2 Structural isomerism :

When two or more organic compounds have same molecular formula but different structural formula, (i.e., they differ in connectivity of atoms) then they are called **structural isomers** and the phenomenon is called structural isomerism

Structural isomers have always different IUPAC name

Ex. $CH_3-CH=CH-CH_3$ (But – 2 – ene), $CH_3CH_2CH=CH_2$ (But – 1 – ene)] structural Isomers

Ex. $CH_3-CH(CH_3)-CH_2-CH_3$ (2 – Methyl butane), $CH_3-CH(CH_3)-CH_2CH_3$ (2 – Methylbutane)] Identical compounds (not isomers)

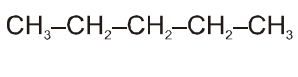
10.3 Various types of structural isomers are :

D5:

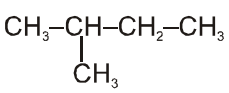
(a) **Chain isomerism:** Compounds having same molecular formula but different carbon skeletons (either difference in main chain or side chain) are known as chain isomers & phenomenon is known as chain isomerism.

Condition : They have same nature of locants.

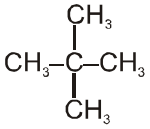
Ex.



(i) Pentane
(Main chain of 5C)

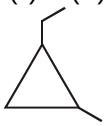


(ii) Isopentane
(Main chain of 4 C)

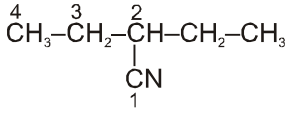
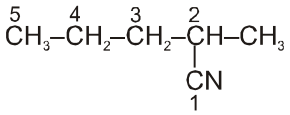


(iii) Neopentane
(Main chain of 3C)

(i), (ii) & (iii) are chain isomers :

Ex. (i)  (ii) 

Size of main chain = 3 | Size of main chain = 3
Size of longest Side chain = 2 | Size of longest side chain = 1
Both are chain isomers due to difference in number of carbon atoms in side chain.

Ex.  & 

2-Ethylbutanenitrile | 2-Methylpentanenitrile

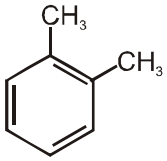
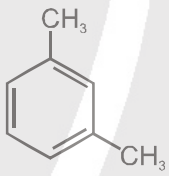
D6:

(b) **Position isomerism :** Compounds have same size of main chain & side chain along with same nature of locants but having different position of locants are known as position isomers & phenomenon is position isomerism.

Ex. $CH_3CH_2CH_2OH$ & $CH_3-\underset{OH}{\underset{|}{CH}}-CH_3$

Propan-1-ol | Propan-2-ol

Difference only in position of –OH group

Ex.  &  & 

o-Xylene | m-Xylene | p-Xylene

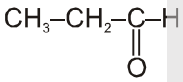
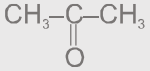
Difference only in position of $-CH_3$ group

D7:

(c) **Functional isomerism :** Compounds having same molecular formula but different functional group are known as functional isomers & phenomenon is functional isomerism.

Ex. CH_3-O-CH_3 & CH_3-CH_2-OH

Methoxymethane | Ethanol

Ex.  & 

Propanal | Propanone

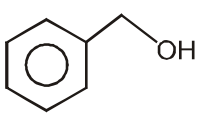
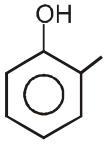
Ex. $CH_3-CH=CH-CH_3$ & 

But-2-ene | Cyclobutane

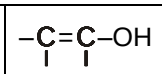
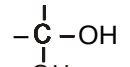
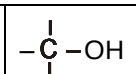
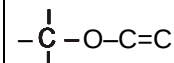
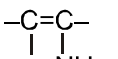
It is also known as **ring chain isomerism** [as 1 isomer has ring & another has aliphatic chain]

Note :

(1) 1º, 2º, 3º amines are functional isomers.
(2) 1º, 2º, 3º amides are functional isomers.
(3) Alcohol attached to sp^2 C is chemically different from alcohol attached to sp^3 C.

 &  are functional isomers.

(4) Following compounds don't exist at room temperature therefore not considered as a structural isomer.

(i)		(ii)	–C≡C–OH	(iii)		(iv)	
(v)		(vi)	Any peroxy compound	(vii)			

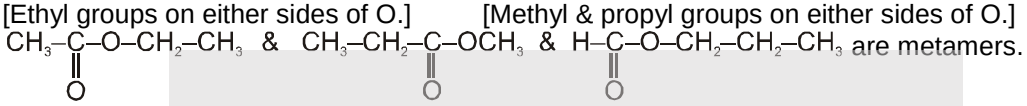
D8:

(d) **Metamerism :** Compounds having same nature of functional groups but different nature of alkyl groups along that polyvalent functional group are known as metamers & phenomenon is metamerism.

Ex. $CH_3–CH_2–O–CH_2–CH_2$ & $CH_3–O–CH_2–CH_2–CH_3$

Ethoxy ethane — Methoxy propane

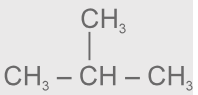
[Ethyl groups on either sides of O.] — [Methyl & propyl groups on either sides of O.]

Ex.  are metamers.

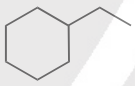
Ex.  are metamers.

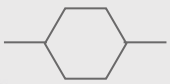
Ex. Identify relationship between the given compounds :

(a) (i) $CH_3–CH_2CH_2–CH_3$
Butane
Size of main chain = 4
Size of side chain = 0

(ii) 
2-Methylpropane
Size of main chain = 3
Size of side chain = 1

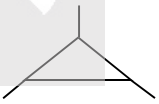
Structure (i) & (ii) are chain isomers.

(b) (i) 
1–Ethylcyclohexane
Size of main chain = 6
Size of side chain = 2

(ii) 
1,4-Dimethylcyclohexane
Size of main chain = 6
Size of side chain 1 = 1
Size of side chain 2 = 1

Structure (i) & (ii) are chain isomers.

(c) (i) 
Cyclohexane
Size of main chain = 6
Size of side chain = 0

(ii) 
1,2,3–Trimethylcyclopropane
Size of main chain = 3
Size of side chain 1 = 1
Size of side chain 2 = 1
Size of side chain 3 = 1

Structure (i) & (ii) are chain isomers.

(d) $\left.\begin{matrix} H_3C-CH_2-CH=CH_2 & (but-1-ene) \\ H_3C-CH=CH-CH_2 & (but-2-ene) \end{matrix}\right]$ position isomers

(e) $\left.\begin{matrix} HC\equiv C-CH_2-CH_2-CH_3 & (pent-1-yne) \\ H_3C-C\equiv C-CH_2-CH_3 & (pent-2-yne) \end{matrix}\right]$ position isomers

(f) (i) $CH_3–CH_2OH$ (Ethanol)
Functional groups –OH
Structure (i) & (ii) are functional isomers.

(ii) $CH_3–O–CH_3$ (Methoxymethane)
Function groups –O–

(iii) $CH_3 – \overset{\overset{O}{\|}}{C} – OH$
Ethanoic acid

Functional groups –COOH
Structure (iii) & (iv) are functional isomers.

(iv) $H – \overset{\overset{O}{\|}}{C} – OCH_3$
Methyl methanoate

Functional groups $– \overset{\overset{O}{\|}}{C} – O –$

(g) (i) $C_2H_5–O–C_2H_5$ (Diethyl ether)
Hydrocarbon groups $–C_2H_5$, $–C_2H_5$
Structure (i) & (ii) are metamers.

(ii) $C_3H_7–O–CH_3$ (Methyl propyl ether)
Hydrocarbon groups $–C_3H_7$, $–CH_3$