# **IUPAC NOMENCLATURE & STRUCTURAL ISOMERISM**



- Que. Calculate  $\sigma$  and  $\pi$  bond in following compounds. (a) HC = CCH=CHCH<sub>3</sub> (b) CH<sub>2</sub> = C = CHCH<sub>3</sub>
- **Sol.** (a) σc-c: 4 ; σc-H : 6 ; πc=c : 1 ; πc=c : 2 (b) σc-c: 3 ; σc-H : 6 ; πc=c : 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<sub>2</sub>.

## Th2: 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.



Que. Expand each of the following condensed formulas into their complete structural formulas. (a)  $CH_3CH_2COCH_2CH_3$  (b)  $CH_3CH=CH(CH_2)_3CH_3$ 



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

(a) HOCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH(CH<sub>3</sub>)CH(CH<sub>3</sub>)CH<sub>3</sub>

Sol. Condensed formula :

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



OH

(b)  $N \equiv C - CH - C \equiv N$ 

(b) HOCH(CN)<sub>2</sub>

#### Th3: 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  $\pi$  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)



Where n = number of carbon atoms in the molecule



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 :

#### 5.1 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	$n = 2 \Longrightarrow C_2 H_6$	-	Ethane
$n = 3 \Rightarrow CH_3CH_2CH_3$	_	Propane	$n = 4 \Rightarrow CH_3CH_2CH_2CH_3$	_	Butane
$n = 5 \Rightarrow CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2$	з —	Pentane	$n = 10 \Rightarrow CH_3(CH_2)_8CH_3$	-	Decane

## 5.2 Alkenes [general formula C<sub>n</sub>H<sub>2n</sub> 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.

				CH <sub>3</sub>
Ex.	CH <sub>2</sub> =CH <sub>2</sub>	CH <sub>3</sub> –CH=CH <sub>2</sub>	CH <sub>3</sub> –CH <sub>2</sub> –CH=CH <sub>2</sub>	$CH_3 - \dot{C} = CH_2$
	ethylene	propylene	butylene	Isobutylene

## 5.3 Alkynes [general formula C<sub>n</sub>H<sub>2n-2</sub> 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=CH – Acetylene CH<sub>3</sub>-C=CH – Methyl acetylene CH<sub>3</sub>-C=C-CH(CH<sub>3</sub>)<sub>2</sub> – Ethylacetylene



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.** 
$$CH_3CH_2CH_2-COOH$$

Residue Functional Group

## Section (B) : IUPAC-Nomenclature of Alkane & Cycloalkane Th6: 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

#### 6.1 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	lcos
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

#### 6.2 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

## 6.3 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	<ul> <li>– oic acid (carboxylic acid)</li> </ul>	Carboxy
2.	R – SO₃H	Alkane sulphonic Acid	– sulphonic acid	sulpho
3.	R-C-O-C-R       O O	Alkanonic Anhydride	– oic anhydride (carboxylic anhydride)	
4.	R – COOR	Alkyl alkanoate	<ul> <li>– oate (carboxylate)</li> </ul>	alkoxy carbonyl or alkanoyl oxy
5.	R – C – X	Alkanoyl halide	–oyl halide (carbonyl halide)	halo carbonyl

	-			
	0			
6.	R – C – NH2    O	Alkanamide	– amide (carboxamide)	carbamoyl
7.	$R - C \equiv N$	Alkanenitrile	<ul> <li>– nitrile (carbonitrile)</li> </ul>	cyano
8.	R – C – H    O	Alkanal	– al (carbaldehyde)	formyl / oxo
9.	R – C – R    O	Alkanone	– one	охо
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 <sub>3</sub> CH <sub>2</sub> OH	Eth	an(e)	ol	Ethanol
$CH_3CH_2CH_2NH_2$	Prop	an(e)	amine	Propanamine
CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> COOH	But	an(e)	oic acid	Butanoic acid
CH₃CH₂CN	Prop	an(e)	nitrile	Propanenitrile
CH <sub>2</sub> =CHCHO	Prop	en(e)	al	Propenal
$HC \equiv CCOOH$	Prop	yn(e)	oic acid	Propynoic acid

## 6.4 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, CH<sub>2</sub>

#### Ex.

 $\begin{array}{cccc} \dot{CH}_2 & \dot{CH}_2 & Cyclo + pent + ane = Cyclopentane \\ & & \\ & & \\ CH_2 & - CH_2 \end{array}$ 

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

## 6.5 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 <sub>3</sub> (–OMe)	Methoxy
– Cl	Chloro	$-OC_2H_5(-OEt)$	Ethoxy
– Br	Bromo	– R	Alkyl
– I	lodo	– CH₃ (–Me)	Methyl
- NO2	Nitro	– C₂H₅ (–Et)	Ethyl
– NO	Nitroso	– CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> (n-Pr)	n-Propyl
$-\stackrel{\oplus}{N}\equiv N$	Diazo	- CH(CH <sub>3</sub> ) <sub>2</sub> (-iPr)	Isopropyl
– OR	Alkoxy	– C(CH <sub>3</sub> ) <sub>3</sub> (t-Bu)	t-Butyl

	Example :				
	Organic compounds	Secondary prefix	Word root	Primary suffix	IUPAC name
	CH <sub>3</sub> CH <sub>2</sub> – Br	Bromo	eth	ane	Bromoethane
	$CH_3 - NO_2$	Nitro	meth	ane	Nitromethane
	$C_2H_5 - OC_2H_5$	Ethoxy	eth	ane	Ethoxyethane
Ex. $ \begin{array}{ccccccccccccccccccccccccccccccccccc$				1-ol Secondary suffix ane <sub>+</sub> 1-sulp Primary S suffix S	ohonic acid econdary suffix
	Word root Primary suffix Secondary suffix	= = =	nex an(e) ol		
<b>Th7:</b> <sup>7.1</sup>	IUPAC nomenciat Parent carbon chain se	ure of brand lection :	ched / com	olex alkanes	i

#### Th 7.1

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

CH₃ CH₂

 $CH_3 - \dot{C} - \dot{C}H_2 - \dot{C}H_2 - \dot{C}H_3$  longest chain has 7 carbons so word root is "Hept"  $\overset{1}{\mathrm{C}}\mathrm{H}_{2}-\overset{2}{\mathrm{C}}\mathrm{H}_{2}-\overset{1}{\mathrm{C}}\mathrm{H}_{3}$ 

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

$$CH_3 - H_2C - CH - CH - CH_3$$
  
 $CH - CH_2 - CH_2 - CH_3$   
 $CH_2 - CH_2 - CH_3$   
 $CH_2 - CH_2 - CH_3$   
 $CH_2 - CH_2 - CH_3$ 

(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.





Chain- (B) 1'-2'-3'-4-5-6-7-8 Chain- (A) 1-2-3-4-5-6-7-8 Chain- (A) & Chain- (B) both have 2 substituents but in chain-B substituent is nearer (at 2<sup>nd</sup> position) than in chain-A (at 3<sup>rd</sup> 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 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.

#### 7.2 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 :

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

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

6 CH

Ex. (i) 
$$CH_{3} - H_{2}C - \dot{C}H - \dot{C}H - \dot{C}H_{3}$$
  
 $\dot{C}H - \dot{C}H_{2} - \dot{C}H_{3}$   
 $\dot{C}H_{2} - CH_{2} - \dot{C}H_{3}$   
(ii)  $CH_{3} - H_{2}C - \dot{C} - \dot{C}H - \dot{C}H_{3}$   
 $\dot{C}H_{2} - CH_{2} - \dot{C}H_{3}$   
 $\dot{C}H_{2} - \dot{C}H_{2} - \dot{C}H_{3}$   
 $\dot{C}H_{2} - \dot{C}H_{2} - \dot{C}H_{3}$   
 $\dot{C}H_{2} - CH_{2} - \dot{C}H_{3}$   
 $\dot{C}H_{2} - CH_{2} - CH_{3}$   
(iii)  $H_{3}C - H_{C}^{2} - H_{C}^{3} - H_{C}^{4} - H_{2}^{5} - \dot{C}H_{3}$   
 $\dot{C}H_{3} - H_{2}^{2} - CH_{3}$   
 $\dot{C}H_{3} - \dot{C}H_{2} - CH_{3}$   
 $\dot{C}H_{3} - \dot{C}H_{2} - \dot{C}H_{3}$ 

3-Ethyl-2-methyl-4-propylheptane

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

3-Ethyl-2,4-dimethylhexane

# Section (C) : IUPAC-Nomenclature of Alkene, Cycloalkene, Polyenes & Alkyne Th8: IUPAC nomenclature of Alkenes/Alkynes/Alkenyne

8.1 Alkenes :

Functional group : --C=C-

(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  $\Rightarrow$  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, 
$$CH_3CH_2CH_2 - CH_2 - CH_2 = CH_2$$
  
4CH<sub>2</sub>  
5CH<sub>2</sub>  
6CH<sub>2</sub>

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

**Ex.**  $\mathring{C}H_3 \qquad \mathring{C}H_3$ **Ex.**  $\mathring{C}H_3 - \mathring{C} - \mathring{C}H = \mathring{C}H - \mathring{C} - \mathring{C}H_3$ , 2,2,5,5-Tetramethylhex-3-ene  $CH_3 \qquad CH_3$ 

#### 8.2 Alkynes

Ex.

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

Ex. CH₃C≡C–CH₃ But-2-yne

 $\dot{C}H_3 - \dot{C} - \dot{C}H_2 - \dot{C} \equiv \dot{C}H$  4,4-Dimethylpent-1-yne  $\dot{C}H_3$ 

## 8.3 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.

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

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.



(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

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

Cyclohexylbenzene

2-Propylcyclohexan-1-ol

(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. OH



Ex.



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.

		<u> </u>	
Fun	Functional Group Suffix		ıffix
СНО		Carbaldehyde	
	СООН	Carbox	ylic Acid
	COX	Carbon	ıyl halide
	COOR	Alkyl Ca	rboxylate
	CONH <sub>2</sub>	Carbo	xamide
	CN	Carbonitrile	

Ex.

Cyclohexanecarbonitrile

соон

2-Cyclohexyl ethanoic acid

СНО Cyclohexanecarbaldehyde COOC<sub>2</sub>H<sub>5</sub>

Ethyl 2-oxocyclohexane-1-carboxylate



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.  $HO - CH_2 - CH_2 - O_1$ 

Ex.

 $HO - CH_2 - CH_2 - O'$ 

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



#### 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.



#### 10.3 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<sub>2</sub>) and alkoxy (-OR) are always treated as substituent groups. NH<sub>2</sub>

5 СН<sub>3</sub> -

$$\begin{array}{c|c} 4 & 2 & 1 \\ -CH - CH - CH - CH - CH_{3} \\ & | & | \\ CI & OH \end{array}$$

4-Amino-3-chloropentan-2-ol (- NH<sub>2</sub> & - CI group treated as substituent) Numbering the principal chain order is

[Principal functional group > double bond > triple bond > substituents] Ο 0

5

⊿اا 3

Ex.

$$\begin{array}{c} \mathsf{CH}_{3}-\overset{II}{\mathsf{C}}-\mathsf{CH}_{2}-\mathsf{COOH}\\ 3\text{-Oxobutan-1-oic acid}\\ [-\operatorname{COOH}>-\operatorname{CO}] \\ \mathsf{O}=\overset{6}{\mathsf{CH}}-\overset{5}{\mathsf{CH}}_{2}-\overset{4}{\mathsf{CI}}-\overset{3}{\mathsf{C}}+\overset{2}{\mathsf{C}}+\overset{1}{\mathsf{CH}}_{2}-\overset{1}{\mathsf{CH}}\\ -\overset{6}{\mathsf{CH}}-\overset{6}{\mathsf{CH}}_{2}-\overset{1}{\mathsf{COH}}\\ \mathsf{O}=\overset{6}{\mathsf{CH}}-\overset{5}{\mathsf{CH}}_{2}-\overset{4}{\mathsf{CH}}_{2}-\overset{3}{\mathsf{C}}-\overset{1}{\mathsf{CH}}_{2}-\overset{1}{\mathsf{COOH}}\\ 3, 6\text{-Dioxohexanoic acid or 5-Formyl-3-oxopentanoic acid}\\ [\operatorname{COOH}>C \& \operatorname{CHO}] \\ \mathsf{H}\end{array}$$

- (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)  $HOOC CH_2 CH_2 COOH_4$

Butane-1, 4-dioic acid

(b) 
$$\begin{array}{c} 1 & 2 & 3 & 4 & 5 \\ NC - CH - CH - CH_2 - CH_2 - CH_2 - CN_1 \\ \\ CH_3 \\ 2 - Methylpen tanedinitrile \end{array}$$

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

Parent chain contains five rather than six carbon atoms.

## Section (F) : IUPAC-Nomenclature of Aromatic compounds Th11: 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	CH <sub>3</sub>	Xylene (o,m,p)	(o,m,p) Dimethylbenzene	
	3	CH <sub>3</sub> CH <sub>3</sub> CH <sub>3</sub>	Mesitylene	1,3,5-Trimethylbenzene	
	4	CH(CH <sub>3</sub> ) <sub>2</sub>	Cumene	lsopropylbenzene	
	5		Styrene	Phenyl ethane or Ethenylbenzene	
	6	$\bigcirc \bigcirc \bigcirc$	Naphthalene	Naphthalene	
	7	$\bigcirc \bigcirc $	Anthracene	Anthracene	
	8		Phenanthrene	Phenanthrene	
	9		Pyrene	Pyrene	
		Aromatic Alcohols			
	10	5- O	Carbolic acid	Phenol	
	11		(o, m, p) cresol	Methylphenol	
	12	ОН	Catechol	Benzene-1,2-diol	

13	ОН	Resorcinol	Benzene-1,3-diol	
14	ОН	Hydroquinone (Quinol)	Benzene-1,4-diol	
15	OH O	$\alpha$ -Naphthol	Naphthalen-1-ol	
16		β-Naphthol	Naphthalen-2-ol	
17		Oil of bitter almonds	Benzenecarbaldehyde	
18	СНООН	Salicylaldehyde	2-Hydroxybenzaldehyde (2-Hydroxybenzene carbaldehyde)	
19	СНОСНО	Phthalaldeyde	Benzene-1,2-dicarbaldehyde	
20	GH <sub>2</sub> -CH <sub>2</sub> -CHO	β- phenylpropionaldehyde	3-Phenylpropanal	
	Aromatic Ketones			
21	C - CH3	Acetophenone	Acetophenone	
22		Bennzophenone	Benzophenone (Diphenylketone)	
23		Phenacyl chloride	Chloroacetophenone	
	Aromatic Acids			
24	COOH	Benzoic acid	Benzenecarboxylic acid (Benzoic acid)	
25		o-toluic acid	2-Methylbenzenecarboxylic acid	

IUPAC Nomenclature and Structural Isomerism					
26	CH = CH – COOH	Cinnamic acid	3–Phenylprop–2–enoic acid		
27	ососн <sub>3</sub>	Aspirin (Acetyl salicylic acid)	2- Ethanolyoxybenzenecarboyxlic acid		
28	СООН	Pthalic acid	Benzene 1,2-dicarboxylic acid		
29	СООН	Terephthalic acid	Benzene 1,4–dicarboxylic acid		
30	ОН	Salicylic acid	2-Hydroxybenzene carboxylic acid		
	Aromatic Ethers				
31		Anisole	Methoxybenzene		
32		Phenetol	Ethoxybenzene		
33		Diphenyl ether	Phenoxybenzene		
	Aromatic Nitro Compounds				
34		Oil of mirbane	Nitrobenzene		
35		_	1,3-Dinitrobenzene (m-Dinitrobenzene)		
36		Picric acid	2,4,6-Trinitrophenol		

	$O_{3}N \setminus A > NO_{3}$			
37		_	2,4,6-Trinitrotoluene(TNT)	
07			An explosive	
	Aromatic Amines			
	NUL			
38		Aniline	Aniline (Benzenamine)	
	$\begin{bmatrix} NH_2 & NH_2 & NH_2 \\ I & I & I \end{bmatrix}$			
39		(o, m, p) Toluidine	Methylaniline	
	CH,			
40		o-Phenylenediamine	Benzene-1,2-diamine	
41	$\widehat{\Box}$	N,N–Dimethylaniline	N,N–Dimethylbenzenamine	
	$\bigcirc$			
	Aromatic Alkyl Amines			
	Aromatic Alkyl Amines CH,NH,			
42	Aromatic Alkyl Amines	Benzylamine	Phenylmethanamine	
42	Aromatic Alkyl Amines	Benzylamine	Phenylmethanamine	
42	Aromatic Alkyl Amines $CH_2NH_2$ $\beta$ $\alpha$	Benzylamine	Phenylmethanamine	
42	Aromatic Alkyl Amines $CH_2NH_2$ O $CH_2NH_2$ O O O O O O O O	Benzylamine	Phenylmethanamine	
42	Aromatic Alkyl Amines $CH_2NH_2$ $CH_2NH_2$ $CH_2-CH_2-NH_2$ $CH_2-CH_2-NH_2$	Benzylamine β-Phenyl ethyl amine	Phenylmethanamine 2-Phenylethanamine	
42	Aromatic Alkyl Amines $H_2NH_2$ G G G G G G G G	Benzylamine β-Phenyl ethyl amine	Phenylmethanamine 2-Phenylethanamine	
42	Aromatic Alkyl Amines $CH_2NH_2$ $O$	Benzylamine β-Phenyl ethyl amine	Phenylmethanamine 2-Phenylethanamine	
42	Aromatic Alkyl Amines $G_{H_2}NH_2$ $G_{H_2}-CH_2-NH_2$ $G_{H_2}$	Benzylamine β-Phenyl ethyl amine	Phenylmethanamine 2-Phenylethanamine	
42	Aromatic Alkyl Amines $CH_2NH_2$ $O$ $CH_2-CH_2-NH_2$ $O$ $CH_2-CH_2-NH_2$	Benzylamine β-Phenyl ethyl amine	Phenylmethanamine 2-Phenylethanamine	
42 43 43 44	Aromatic Alkyl Amines $GH_2NH_2$ $GH_2-CH_2-NH_2$	Benzylamine β-Phenyl ethyl amine Benzamide	Phenylmethanamine 2-Phenylethanamine Benzenecarboxamide	
42 43 44	Aromatic Alkyl Amines $G_{H_2}NH_2$ $G_{H_2}-CH_2-NH_2$	Benzylamine β-Phenyl ethyl amine Benzamide	Phenylmethanamine 2-Phenylethanamine Benzenecarboxamide	
42 43 44	Aromatic Alkyl Amines $G_{H_2}NH_2$ $G_{H_2}-CH_2-NH_2$ $G_{H_2}-CH_2-NH_2-NH_2$ $G_{H_2}$	Benzylamine β-Phenyl ethyl amine Benzamide	Phenylmethanamine 2-Phenylethanamine Benzenecarboxamide	
42 43 44	Aromatic Alkyl Amines $GH_2NH_2$ $GH_2NH_2$ $GH_2-CH_2-NH_2$ $GH_2-CH_2-NH_2-H_2$ $GH_2-CH_2-NH_2-H_2$	Benzylamine β-Phenyl ethyl amine Benzamide	Phenylmethanamine 2-Phenylethanamine Benzenecarboxamide	
42 43 44 44	Aromatic Alkyl Amines $G_{H_2NH_2}$ $G_{H_2-CH_2-NH_2}$ $G_{H_2-CH_2-NH_2-NH_2}$ $G_{H_2-NH_2-NH_2-NH_2-NH_2-NH_2-NH_2-NH_2-N$	Benzylamine β-Phenyl ethyl amine Benzamide	Phenylmethanamine 2-Phenylethanamine Benzenecarboxamide	
42 43 44 45	Aromatic Alkyl Amines $G_{H_2}NH_2$ $G_{H_2}-CH_2-NH_2$ <	Benzylamine β-Phenyl ethyl amine Benzamide	Phenylmethanamine 2-Phenylethanamine Benzenecarboxamide N-Phenylethanamide	
42 43 44 45	Aromatic Alkyl Amines $G_{H_2NH_2}$ $G_{H_2-CH_2-NH_2}$ $G_{H_2-NH_2-NH_2}$ $G_{H_2-NH_2-NH_2-NH_2}$ $G_{H_2-NH_2-NH_2-NH_2-NH_2-NH_2-NH_2-NH_2-N$	Benzylamine β-Phenyl ethyl amine Benzamide Acetanilide	Phenylmethanamine 2-Phenylethanamine Benzenecarboxamide N-Phenylethanamide	

46	$\begin{array}{c} C_6H_5-C-O-C-C_6H_5\\ \parallel & \parallel\\ O & O\end{array}$	Benzoic anhydride	Benzenecarboxylic anhydride	
	Aromatic Esters			
47	$H_3C_4$ $O-C_1-CH_3$	_	4–Methylphenyl ethanoate	
48	OH COOCH3	Oil of winter green (Methyl salicylate)	Methyl-2-hydroxy benzenecarboxylate	
	Arenediazonium Salts			
49	$\bigwedge^{\oplus}_{N} = NHSO_4^{\ominus}$	_	Benzene diazonium hydrogen sulphate	
50	$\bigwedge \bigoplus N \equiv NCl^{\Theta}$	_	Benzene diazonium chloride	
51		_	Azobenzene	

Write IUPAC name of following aromatic compounds Que. CH₃



(c) 2,3-Dibromo-1-phenylpentane



- (b) p-Nitroaniline,
- (d) 4-Ethyl-1-fluoro-2-nitrobenzene.



## Common and IUPAC Names of Some Organic Compounds

		O a margan Nama a	
S.NO.	Compound	Common Names	IUPAC Name
	$CH_2 - Br$		
1		Ethylene dibromide	1,2-Dibromoethane
	ĊH <sub>2</sub> – Br		
2		Ethylidana bramida	1.1 Dibromoothono
2	 Br	Ethylidene bromide	I, I-Dibromoethane
	Ы		
3	CH≡C–CH₂–OH	Propargyl alcohol	Prop-2-yn-1-ol
	$CH_{3} - CH - CH_{3}$		
4		Propylene alvcol	Propane-1.2-diol
-	ÓH ÓH	3,9,000	
5		Trimethylene glycol	Propane-1.3-diol
5			
	$CH_2 - CH - CH_2$		
6		Glycerol or Glycerine	Propane-1,2,3-triol
7	H–CHO	Formaldehyde	Methanal
8	CH₃–CHO	Acetaldehyde	Ethanal
9	CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> -CHO	n-Butvraldehvde	Butanal
-			
10	сн – сно	Isobutvraldehvde	2-Methylpropanal
	CH	loobadyraidollydd	
11		Acrolein	Propenal
12		Crotonaldobydo	Rut 2 opol
12	CH3CH=CH-CHO		Dut-2-enai
13	CH <sub>3</sub> –CO–CH <sub>3</sub>	Dimethyl ketone or	Propanone
		Acetone	
14	CH <sub>3</sub> –CO–CH <sub>2</sub> CH <sub>3</sub>	Ethyl methyl ketone	Butanone
15	CH <sub>3</sub> –CO–CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>	Methyl n-propyl ketone	Pentan-2-one
16	CH <sub>3</sub> CH <sub>2</sub> –CO–CH <sub>2</sub> CH <sub>3</sub>	Diethyl ketone	Pentan-3-one
17	CH <sub>3</sub> CO–CH=CH <sub>2</sub>	Methylvinyl ketone	But-3-en-2-one
18	H-COOH	Formic acid	Methanoic acid
10		Acetic acid	Ethanoic acid
20		n Buturio goid	Putanoia agid
20			Dutanoic aciu
21		n-valeric acid	Pentanoic acid
22		Iso-butyric acid	2-Methylpropanoic acid
23	CH <sub>2</sub> =CH–COOH	Acrylic acid	Propenoic acid
	COOH		
24		Oxalic acid	Ethanedioic acid
	СООН		
	СООН		
25	H <sub>2</sub> C	Malonic acid	Propanedioic acid
	_соон		
	H <sub>2</sub> C – COOH		
26		succinic acid	Butanedioic acid
	$H_2C = COOH$		
27	H <sub>2</sub> C	Glutaric acid	Pentanedioic acid
	Н		
28	H₃C−Ċ−COOH	Lactic acid	2-Hydroxypropanoic acid
	OH		
	0		
29		Pyruvic acid	2-Oxopropanoic acid
	H <sub>3</sub> C-C-COOH	-	

30	носнсоон   носнсоон	Tartaric acid	2,3–Dihydroxybutane dioic acid
31	Н <sub>2</sub> С – СООН  ОН ССООН   СН <sub>2</sub> – СООН	Citric acid	2-Hydroxypropane-1-2,3-tricarboxylic acid
32	HO – CH – COOH   CH₂COOH	Malic acid	2-Hydroxy-butanedioic acid
33		Maleic acid	cis-But-2-enedioic acid
34		Fumaric acid	trans-But-2-enedioic acid
35	CH <sub>2</sub> =CH–COOH	Acrylic acid	Propenoic acid
36	H₃C–CH=CH–COOH	Crotonic acid	But-2-enoic acid
37	H–COOCH <sub>3</sub>	Methyl formate	Methyl methanoate
38	H–COOC <sub>2</sub> H <sub>5</sub>	Ethyl formate	Ethyl methanoate
39	CH <sub>3</sub> -COOC <sub>2</sub> H <sub>5</sub>	Ethyl acetate	Ethyl ethanoate
40	H–COCI (unstable)	Formyl chloride	Methanoyl chloride
41	CH <sub>3</sub> –COCI	Acetyl chloride	Ethanoyl chloride
42	(CH <sub>3</sub> CO) <sub>2</sub> O	Acetic anhydride	Ethanoic anhydride
43	(CH <sub>3</sub> CH <sub>2</sub> CO) <sub>2</sub> O	Propionic anhydride	Propanoic anhydride
44	H–CONH <sub>2</sub>	Formamide	Methanamide
45	CH <sub>3</sub> –CONH <sub>2</sub>	Acetamide	Ethanamide
46	CH <sub>3</sub> CH <sub>2</sub> CONH <sub>2</sub>	Propionamide	Propanamide
47	CH <sub>3</sub> -O-N=O	Methyl nitrite	Methyl nitrite
48	CH <sub>3</sub> CH <sub>2</sub> –O–N=O	Ethyl nitrite	Ethyl nitrite
49	H <sub>2</sub> N–SO <sub>3</sub> H	Sulphamic acid	Aminosulphonic acid
50	CH3-CN	Methyl cyanide or Acetonitrile	Ethanenitrile
51	$O \xrightarrow{H_2C - CH_2} O \xrightarrow{H_2C - H_2C} O$	Dioxane	1, 4-Dioxacyclohexane
52	$ \begin{array}{c}                                     $	Trioxane	1,3,5-Trioxacyclohexane
53		(Gammexane or Lindane or 666) BHC [Benzene hexachloride]	Hexachlorocyclohexane

IUPAC Nomenclature and Structural Isomerisn	n j
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54	CH <sub>3</sub> –N⁺≡C⁻	[Methyl isocyanide or Methyl carbyl amine]	Methane isocyanide
55	NH NH	Barbituric acid	_
56		Ascorbic acid	_

## Th12: Some important 1993 recommendations for IUPAC nomenclature of organic compounds :

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

CH.

 $CH_3CH_2CH = CH_2$  should be named as but-1-ene CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>OH should be named as propan-1-ol

similarly, a few more examples are given as following :

Cyclopent-2-en-1-ol







2,2-Dimethylpropan-1-ol

2. The locant 1 is often omitted when there is no ambiguity. For example. CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>COOH CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CN

CH<sub>3</sub>CH<sub>2</sub>CHO Propanal

Butanenitrile

Butanoic acid 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.

CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>OH Propan-1-ol

CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub> 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
- Simple prefixes such as methyl, ethyl, chloro, nitro, hydroxy, etc. are arranged alphabetically. (i) The prefixes di, tri, etc. are however not considered for comparison.

**Ex.** 
$$\begin{array}{c} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ CH_{3}CH_{2}CHCH_{2}CHCH_{2}CHCH_{2}CH_{2}CH_{3} \\ | & | \\ CH_{3} & C_{2}H_{5} \end{array}$$
  
5-Ethyl-3-methyl octane 1

1-Bromo-2-chloroethane

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

ŹĦ ĊĦ

Br

**Ex.** 
$$\overset{9}{C}H_{3} - \overset{8}{C}H_{2} - \overset{7}{C}H_{2} - \overset{6}{C}H_{2} - \overset{1}{C}H_{2} - \overset{1}{C}H_{2} - \overset{1}{C}H_{2} - \overset{1}{C}H_{2} - \overset{1}{C}H_{3} = \overset{1}{C}H_{3}$$

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.



1-(1-Chloroethyl)-4-(2-chloroethyl)cyclohexane Here, 1-chloroethyl gets priority over 2-chloroethyl.

# **Structural Isomerism**

## 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: Classification of isomerism



## 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



## 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.



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



(g)

	Functional groups –OH		Function groups -O-	-
	Structure (i) & (ii) are functional is	somers.		
(;;;)	О    СН <sub>3</sub> – С – ОН	(iv.)	0    H – C – OCH,	
(111)	Ethanoic acid	(1V)	Methyl methanoate	
				0
	Functional groups –COOH		Functional groups -	C – O –
	Structure (iii) & (iv) are functional	isomer	S.	
(i)	$C_2H_5-O-C_2H_5$ (Diethyl ether) (	(ii)	C <sub>3</sub> H <sub>7</sub> –O–CH <sub>3</sub> (Methy	l propyl ether)
.,	Hydrocarbon groups -C <sub>2</sub> H <sub>5</sub> , -C <sub>2</sub> H	<b>H</b> 5	Hydrocarbon groups	$-C_{3}H_{7}, -CH_{3}$
	Structure (i) & (ii) are metamers.		, , , , , , , , , , , , , , , , , , , ,	-

# CHECK LIST

	Definitions (D)	
	Definitions (D)	
D1	Catenation	
D2	Homologous series	
D3	Degree of unsaturation	
D4	Isomerism	
D5	Chain isomerism	
D6	Position isomerism	
D7	Functional isomerism	
D8	Metamerism	
	Theories (Th)	
Th1:	Bonding in organic compounds	
Th2:	Structural representation of organic compounds	
Th3:	Degree of unsaturation (DU)	
Th4:	Classification of organic compounds	
Th5:	Organic compounds and functional groups	
Th6:	IUPAC system of nomenclature	
Th7:	IUPAC nomenclature of branched/complex alkane	es
Th8:	IUPAC nomenclature of alkenes/alkynes/alkenyne	•
Th9: Th1(	IUPAC nomenclature of alicyclic compounds D: IUPAC nomenclature of compounds contain	□ ining
	functional groups	
Th1 <sup>4</sup> Th12	I: Nomenclature of aromatic compounds 2: Some important 1993 recommendations for IUPA	
	nomenclature of organic compounds	
Th1:	3: Classification of isomerism	