IUPAC Nomenclature

Introduction :

The compounds which were derived from living organism were called as organic compounds while those from non living matter were known as inorganic compounds. Berzilius thought that organic compounds were produced from their element by laws different from those governing the formation of inorganic compounds. Wohler converted inorganic compound ammonium cyanate (found from non living matters) into urea (an organic compound).

$$NH_4CNO \text{ (ammonium cyanate)} \xrightarrow[\text{in the absence of air}]{\text{heat}} NH_2CONH_2 \text{ (urea)}$$

Other synthesis were: Acetic acid by Kolbe in 1845 and Methane by Berthelot in 1856.

Section (A) : Fundamental of Organic Chemistry

Definitions :

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

(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 one CH_2 group.

(iii) Isomerism : Compounds which have the same molecular formula but differ in physical and chemical properties are called isomers and the phenomenon is called isomerism.

Isomerism can be broadly classified into two categories

(1) Structural isomerism (2) Stereoisomerism

Tetravalency of carbon :

The valency of carbon is four as there are four unpaired electrons in outer most orbit in excited state.

Hybridisation	sp^3	sp^2	sp
Angle	109°28′	120°	180°
Geometry	Tetrahedral	Trigonal planar	Linear
Example	Alkane, Cycloalkane and in saturated part of all organic molecules	Alkenes and other compounds containing C=C, C=O, C=N and C=S	Alkynes and all other compounds containing C≡C and C≡N triple bonds,
Bond	Four-σ	Three-σ + One-π	Two-σ + Two-π
% s character	25	33.3	50
% p character	75	66.7	50
Electronegativity	2.48	2.75	3.25

Types of carbon and hydrogen atoms : There are four types of carbon atoms :

(i) A primary (1°) carbon atom is bonded directly to one other carbon atom.

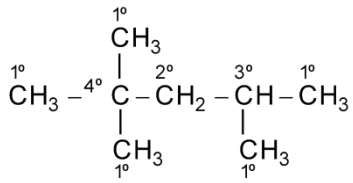
(ii) A secondary (2°) carbon atom is bonded directly to two other carbon atoms.

(iii) A tertiary (3°) carbon atom is bonded directly to three other carbon atoms.

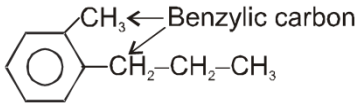
(iv) A quaternary (4°) carbon atom is bonded directly to four other carbon atoms.

The 1°, 2°, 3° and 4° carbon and 1°, 2° and 3° hydrogen atoms are illustrated below :

Ex.



(v) Benzylic carbon [The carbon atom directly attached to the benzene nucleus].



(total benzylic H = 3 + 2 = 5)

(vi) Allylic carbon : The sp^3 carbon atom directly attached with doubly bonded carbon atom.

$CH_2=CH–CH_3$ ← Allylic carbon (Allylic H = 3)

(vii) Vinylic carbon : The sp^2 carbon atom of doubly bonded carbon.

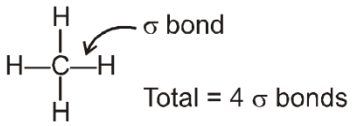
$CH_2=CH_2$ ← Vinylic carbon.

Bonding in organic compounds :

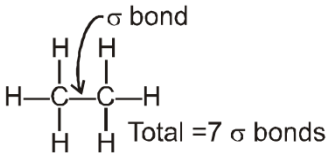
Two types of covalent bond exist in organic compounds.

(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

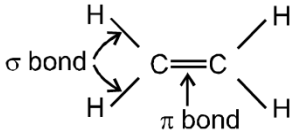


In C_2H_6 molecule



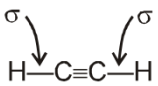
(b) Multiple bond (π) : Any other bond with σ bond is π bond.

Ex. (i) In ethene molecule



Total σ = 5, π = 1

(ii) In ethyne molecule



Total σ = 3, π = 2

Que. Calculate total number of σ and π bonds in following compounds.

(a) $HC \equiv CCH=CHCH_3$ (b) $CH_2 = C = CHCH_3$

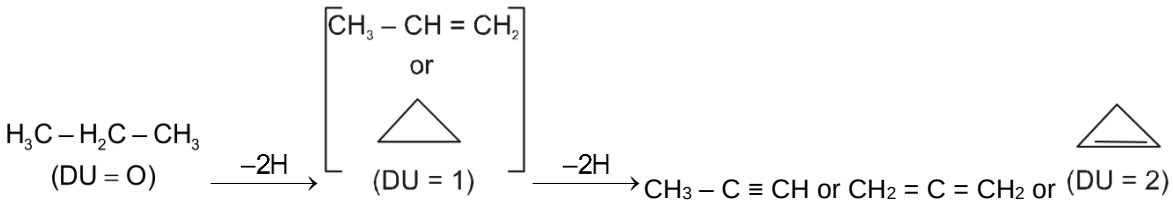
Sol. (a) σ_{C-C} : 4 ; σ_{C-H} : 6 ; $\pi_{C=C}$: 1 ; $\pi_{C\equiv C}$: 2 (b) σ_{C-C} : 3 ; σ_{C-H} : 6 ; $\pi_{C=C}$: 2

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.

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



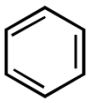
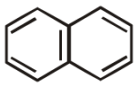
$$\text{Degree of unsaturation (D.U.)} = \frac{(2n+2)-(\text{No. of H atoms}+\text{No. of X atoms}-\text{No. of N atoms})}{2}$$

Where n = number of carbon atoms in the molecule

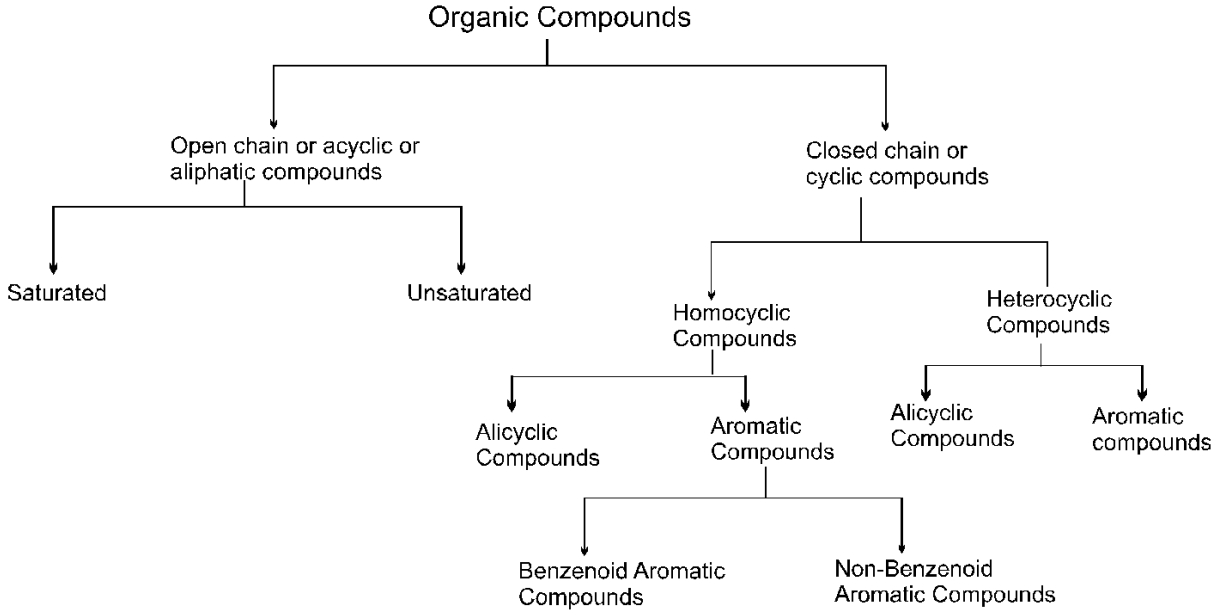
Note : Total no. of cyclic rings + total π−bonds give us degree of unsaturation.

One double bond = one DU, One ring = one DU, One triple bond = two DU

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

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

Section (B) : Classification of organic compounds

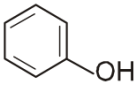


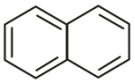
Ex.

(i) Alkanes (Saturated hydrocarbon)	$CH_3–CH_2–CH_3$	Propane
(ii) Alkenes (Unsaturated hydrocarbon)	$CH_3–CH=CH_2$	Propene
(iii) Alkynes (Unsaturated hydrocarbon)	$HC\equiv CH$	Ethyne
(iv) Aliphatic compounds with other functional groups	$CH_3CH_2–OH$	Ethanol (absolute alcohol)
	$CH_3–CH_2–COOH$	Propanoic acid
(v) Homo alicyclic compound		Cyclohexane
(vi) Heteroalicyclic compound		Tetrahydropyran

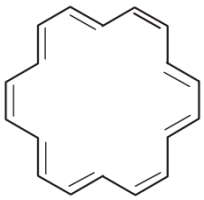
(vii) Homo cyclic benzenoid aromatic compounds  Benzene

(viii) Heterocyclic benzenoid aromatic compound  Pyridine

(ix) Homo cyclic benzenoid aromatic compounds  Phenol



Napthalene



(x) Homo cyclic Non-benzenoid aromatic compound [18] annulene

Organic compounds.

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.

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

These are open–chain aliphatic saturated hydrocarbons 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

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

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

Some names of hydrocarbon groups

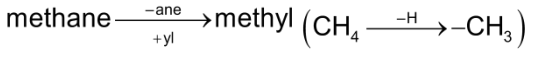
(A) Alkyl, Alkenyl & Alkynyl groups

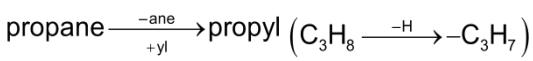
Alkane (C_nH_{2n+2}) $\xrightarrow{-H}$ Alk + yl (C_nH_{2n+1})

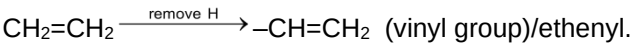
Alkene (C_nH_{2n}) $\xrightarrow{-H}$ Alken + yl (C_nH_{2n-1})

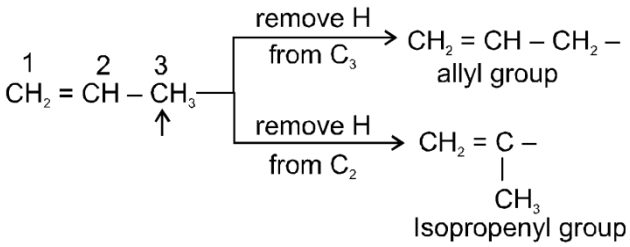
Alkyne (C_nH_{2n-2}) $\xrightarrow{-H}$ Alkyn + yl (C_nH_{2n-3})

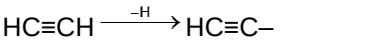
Ex.

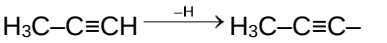


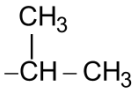




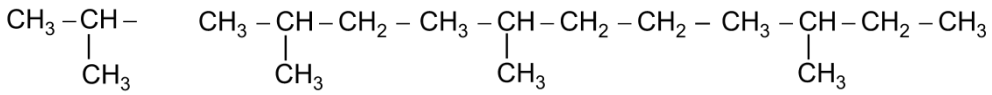




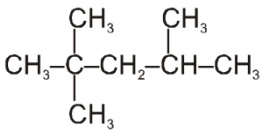


(B) Iso alkyl group : A compound having  group is called iso alkyl group

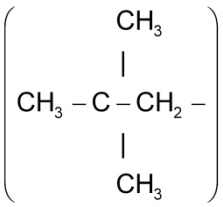
Ex.



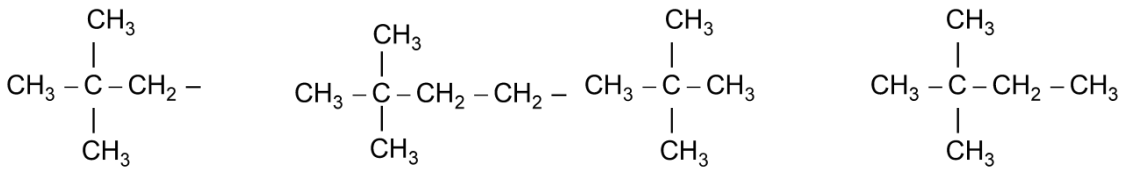
Iso propyl Iso butyl isopentyl Iso pentane



Exception : Isooctane

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

Ex.



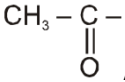
Neopentyl Neohexyl Neopentane Neohexane

(D) Trivial and Derived naming of organic compounds

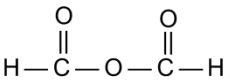
No. of carbon atoms	Word root	–CHO (–aldehyde)	–COOH(–ic acid)	$–CONH_2$ (–amide)	—COOR (–ate)
1	Form	HCHO Formaldehyde	HCOOH Formic acid	$HCONH_2$ Formamide	$HCOOCH_3$ Methyl formate
2	Acet	CH_3CHO Acetaldehyde	CH_3COOH Acetic acid	CH_3CONH_2 Acetamide	CH_3COOCH_3 Methyl acetate
3	Propion	CH_3CH_2CHO Propionaldehyde	CH_3CH_2COOH Propionic acid	$CH_3CH_2CONH_2$ Propionamide	$CH_3CH_2COOCH_3$ Methyl propionate
4	Butyr	$CH_3CH_2CH_2CHO$ n–Butyraldehyde	$CH_3CH_2CH_2COOH$ n–Butyric acid	$CH_3CH_2CH_2CONH_2$ n–Butyramide	$CH_3CH_2CH_2COOH_3$ Methyl n–butyrate
5	Valer	$CH_3(CH_2)_3CHO$ n–Valeraldehyde	$CH_3(CH_2)_3COOH$ n–Valeric acid	$CH_3(CH_2)_3CONH_2$ n–Valeramide	$CH_3(CH_2)_3COOCH_3$ Methyl n–valerate
3C+1 Double bond	Acryl	$CH_2=CH–CHO$ Acrylaldehyde	$CH_2 = CH–COOH$ Acrylic acid	$CH_2=CH–CONH_2$ Acrylamide	$CH_2=CHCOOCH_3$ Methyl acrylate
4C + 1 Double bond (at 2nd Carbon. atom)	Croton	$CH_3–CH=CH–CHO$ Crotonaldehyde	$CH_3CH_2=CH–COOH$ Crotonic acid	$CH_3CH_2=CH–CONH_2$ Crotonamide	$CH_3CH=CHCOOCH_3$ Methyl crotonate

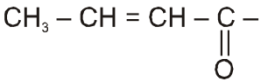
(a) Form group

Ex. HCOOH (formic acid), HCOCl (Formyl chloride), $HCONH_2$ (formamide), (Formic anhydride)



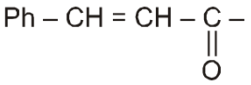
(b) Acet group

Ex. CH_3COOH (Acetic acid), CH_3COCl (Acetyl chloride),  (Acetic anhydride or Ac_2O)



(c) Croton group

Ex.. $CH_3CH=CH–CHO$ (Crontonaldehyde), $CH_3CH=CH–COOH$ (Crotonic acid).



(d) Cinammic group

Ex. PhCH=CH–CHO (Cinammicaldehyde), PhCH=CH–COOH (Cinammic acid).

Section (C) : IUPAC-Nomenclature of Alkane

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

(A) Word root (Alk):

It denotes the number of carbon atoms present in the principal chain (the longest possible continuous chain of carbon atoms including the functional group of an organic compound).

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

(B) 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

(C) Secondary suffix :

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

Class	General IUPAC Name	Suffix	Prefix
1. Carboxylic acid (R–COOH)	Alkanoic Acid	– oic acid (carboxylic acid)	carboxy
2. Sulphonic acid (R–SO_3H)	Alkane sulphonic Acid	– sulphonic acid	sulpho
3. Anhydride (R–CO–O–CO–R)	Alkanoic Anhydride	– oic anhydride (carboxylic anhydride)	----------

4. Ester (R–COOR)	Alkyl alkanoate	– oate (carboxylate)	alkoxy carbonyl
5. Acid halide (R–COX)	Alkanoyl halide	–oyl halide (carbonyl halide)	halo carbonyl
6. Acid amide (R–CONH2)	Alkanamide	– amide (carboxamide)	carbamoyl
7. Cyanide (R–C≡N)	Alkanenitrile	– nitrile (carbonitrile)	cyano
8.Aldehyde (R–CH=O)	Alkanal	– al (carbaldehyde)	formyl / oxo
9. Ketone (R–CO–R)	Alkanone	– one	oxo
10. Alcohol (R–OH)	Alkanol	– ol	hydroxy
11. Thiol (R–SH)	Alkanethiol	– thiol	mercapto
12. Amine ($R–NH_2/R_2NH/R_3N$) (1º/2º/3º Amines)	Alkanamine	– amine	amino

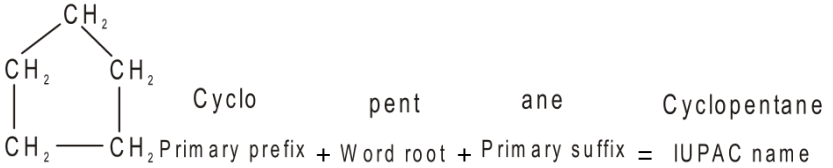
The following examples illustrate the use of word root, primary suffix and secondary suffix in naming of organic compounds.

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

(D) Primary prefix :

A primary prefix is used simply to distinguish between cyclic compounds 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.



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

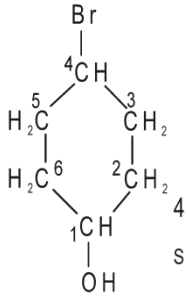
(E) Secondary prefix :

In IUPAC system of nomenclature, certain groups 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

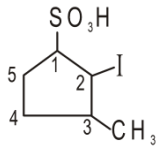
– F	Fluoro	– OCH_3 (– OMe)	Methoxy
– Cl	Chloro	– OC_2H_5(–OEt)	Ethoxy
– Br	Bromo	– R	Alkyl
– I	Iodo	– CH_3 (– Me)	Methyl
– NO_2	Nitro	– C_2H_5 (– Et)	Ethyl
– NO	Nitroso	– $CH_2CH_2CH_3$(n-Pr)	n-Propyl
	Diazo	– $CH(CH_3)_2$ (– iPr)	Isopropyl
– OR	Alkoxy	– $C(CH_3)_3$ (t-Bu)	t-Butyl

Ex.



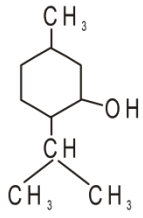
4-Bromo cyclo hex an (e) 1-ol

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

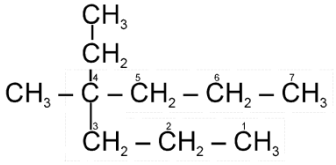


2-Isopropyl-5-methylcyclohexanol(Here : Secondary prefix = 2-Isopropyl-5-methyl)

Primary prefix = cyclo, Word root = hex, Primary suffix = an(e), Secondary suffix= ol

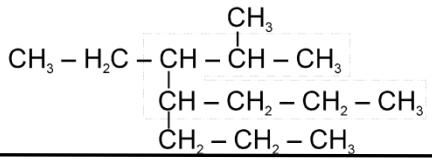
IUPAC nomenclature of branched / complex alkanes

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



Longest chain has 7 carbon atoms so word root is "Hept"

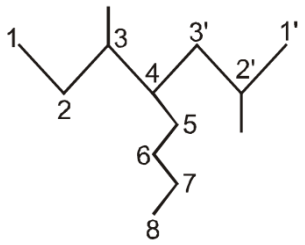
(b) When chains of equal lengths are competing for selection then that chain is selected which has more number of substituents/branches.



longest chain has 7 carbon atoms & 3 substituents

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

Ex. Here , 2 choices for longest chain



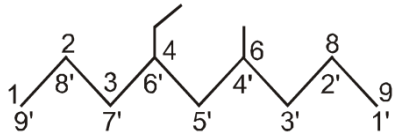
Chain (A) : 1–2–3–4–5–6–7–8
Chain (B) : 1'–2'–3'–4–5–6–7–8

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.

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

(ii) 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.

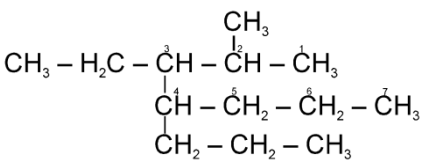
(iii) Prefixes di, tri, tetra etc. are not considered in deciding alphabetical order. for simple substituents but consider for the complex substituents.

(iv) Iso & Neo is consider for alphabetical seniority order.

(v) numbers are separated each other by commas(,).

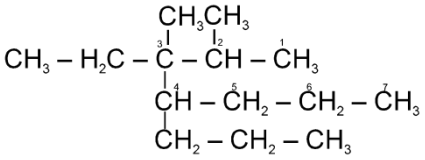
(vi) numbers are separated from words by hyphens and there is no break between name of substituents and word root.

Ex. (i)



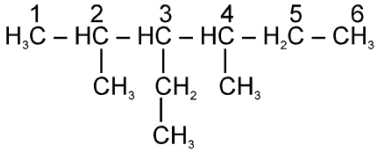
(3–Ethyl–2–methyl–4–propylheptane)

(ii)



(3–Ethyl–2,3–dimethyl–4–propylheptane)

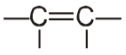
(iii)



(3–Ethyl–2,4–dimethylhexane)

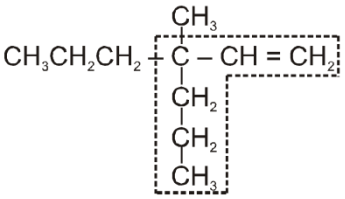
Section (D) : IUPAC-Nomenclature of Alkene, Alkyne & Alkenyne

Alkenes :

Functional group : 

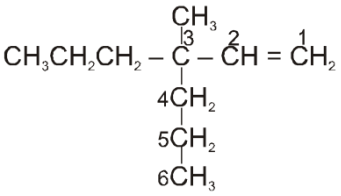
(1) Select the longest carbon chain containing carbon–carbon double bond. This need not be the longest chain in the compound as a whole. Parent name will be alkene corresponding to number of carbon atoms in the longest chain.

Ex.



Longest chain has 6 atoms $\Rightarrow$ parent name = hexene

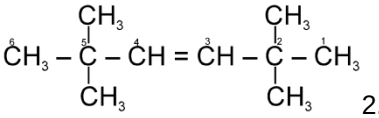
(2) Carbon atoms in the longest chain is numbered from that end in such a way that doubly bonded carbon atom gets the lowest number. The position of double bond is indicated by the smaller of the numbers assigned to two carbon atoms of double bond.



The above example can be numbered as,

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

Ex.

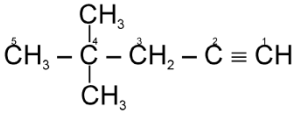


2, 2, 5, 5-Tetramethylhex-3-ene

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



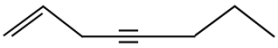
4, 4–Dimethylpent–1–yne

Alkenyne (containing both double and triple bonds)

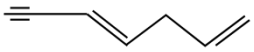
Numbering is done in a manner that double and triple bonds get the lowest possible number. If double bond and triple bond both have same number then double bond is prefer over triple bond.

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

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



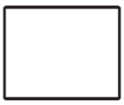
Oct-1-en-4-yne



Hepta-3,6-dien-1-yne

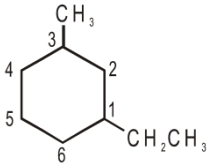
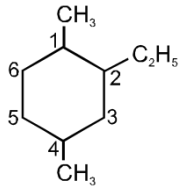
Section (E) : IUPAC-Nomenclature of Cyclic Compounds

(1) The name of alicyclic compound is prefixing by "cyclo".

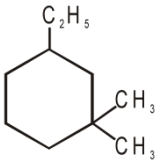
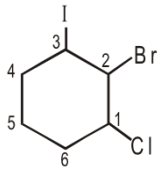
Ex.  

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 allotted the lowest possible number and it does not violate the lowest set of locants rule.

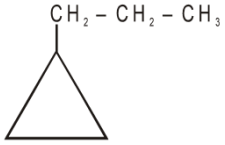
Ex.  

1-Ethyl-3-methylcyclohexane 2-Ethyl-1,4-dimethylcyclohexane

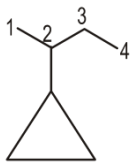
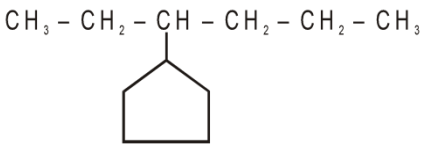
3-Ethyl-1,1-dimethylcyclohexane 2-Bromo-1-chloro-3-iodocyclohexane

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

Ex. 

Propylcyclopropane

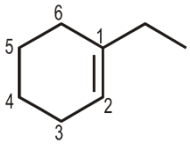
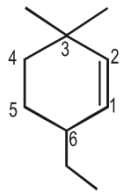
(4) If the alkyl chain contains greater number of carbon atoms than the ring, then the compound is considered as the derivative of alkane and the ring is treated as substituent.

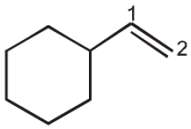
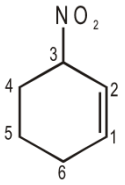
Ex.  

2-Cyclopropylbutane 3-Cyclopentylhexane

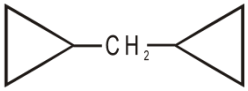
(5) If ring has unsaturation and side chain is saturated then ring is selected as parent chain.
If side chain has unsaturation and ring is saturated then side chain is selected as parent chain.
If both have unsaturation then the chain with maximum unsaturation is selected as parent chain.
If both have 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.

Note : 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

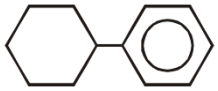
Ex.  1-Ethylcyclohex-1-ene  6-Ethyl-3, 3 -dimethylcyclohex-1-ene

 Cyclohexyl ethene  3-Nitrocyclohex-1-ene

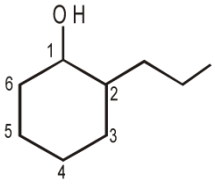
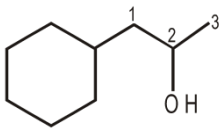
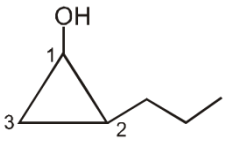
(6) If more than one alicyclic ring is attached to a single chain then the compound is named as a derivative of alkane and the rings are treated as substituent groups.

Ex.  Dicyclopropylmethane

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

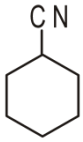
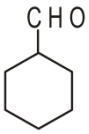
Ex.  Cyclohexylbenzene

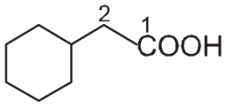
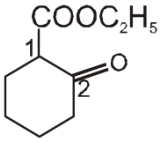
(8) If the functional group is present in the molecule then that chain is consider as parent chain in which senior most functional group is present.

Ex.  2-Propylcyclohexan-1-ol  1-Cyclohexylpropan-2-ol  2-Propyl cyclopropan-1-ol

(9) When chain terminating functional group is directly attached with ring then ring is taken as parent chain & special suffix is used for the following functional groups.

Functional group	Special Suffix	Functional group	Special Suffix
CHO	Carbaldehyde	COOR	Alkyl carboxylate
COOH	Carboxylic acid	$CONH_2$	Carboxamide
COX	Carbonyl halide	CN	Carbonitrile

Ex.  Cyclohexanecarbonitrile  Cyclohexanecarbaldehyde

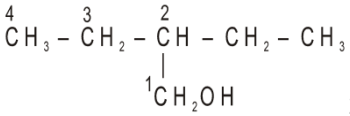
 2-Cyclohexylethanoic acid  Ethyl 2–oxocyclohexane–1–carboxylate

Section (F) : IUPAC - nomenclature of functional groups (–SO_3H, –OH, –NH_2, –SH, C=O)

Rules for non chain terminating functional groups :

(1) **Parent chain :** Select the longest carbon chain with maximum number of principal functional groups and maximum unsaturation without caring whether it is longest chain or not.

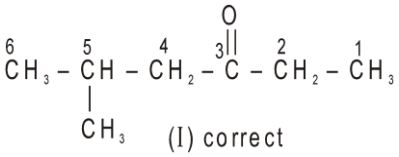
Ex.



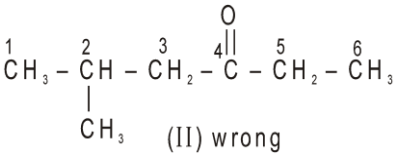
2-Ethylbutan-1-ol (Parent chain contains four rather than five carbon atoms)

(2) **Numbering :** Numbering is done from that end of the chain in which lowest position alloted to the principal functional group followed by double and triple bonds.

Ex.

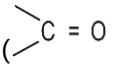


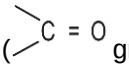
(I) correct



(II) wrong

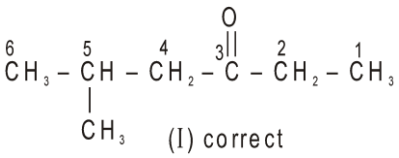
5-Methyl hexan-3-one

( group gets lowest number 3)

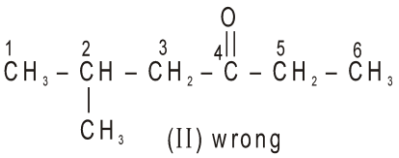
( group gets number 4 which is not lowest)

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

Ex.



(I) correct



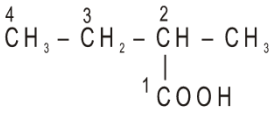
(II) wrong

Section (G & H) : IUPAC-nomenclature of chain terminating functional groups (–COOH, –COOR, –COX, –$CONH_2$, –CN, –CHO, –CO–O–CO–)

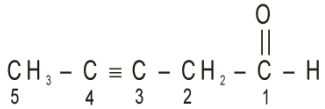
Rules for chain terminating functional groups

(1) When a chain terminating principal functional group such as – CHO, – COOH, – COOR, – $CONH_2$, – COCl, – C ≡ N etc. is present, it is always allotted number 1 (one.)

Ex.

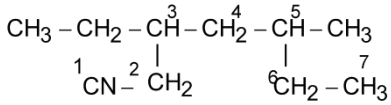


2-Methylbutan-1-oic acid



Pent-3-yn-1-al

Ex.



The longest chain containing functional group is of **7** carbon atoms. Therefore, the word root is hept & the chain is numbered as shown.

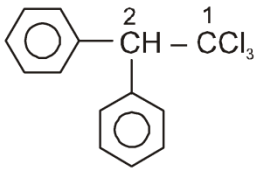
There is no multiple bond in it. Hence, the primary suffix is **ane**.

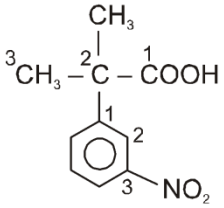
The functional groups is –CN. Hence, secondary suffix is **nitrile**

Moreover, there is a methyl group on carbon 5 and ethyl group on carbon 3.

The IUPAC name is **3-Ethyl-5-methylheptanenitrile**

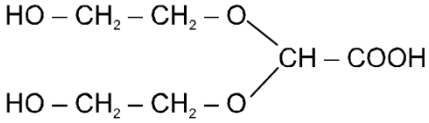
(2) The substituent name for benzene is phenyl. In case the phenyl ring is further substituted, the separate numbering is used for the ring in such a way that the substituent gets the least possible number.





Ex. 1,1,1-Trichloro-2,2-diphenylethane 2-Methyl-2-(3-nitrophenyl) propanoic acid

(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

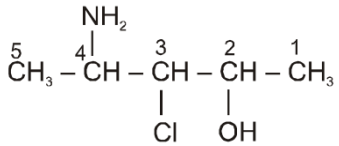
Note : Bis, Tris, tetrakis are not consider for alphabetical seniority order.

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.

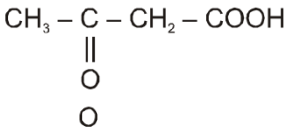
(2) Some functional group such as halo groups (fluoro, bromo, chloro, iodo), nitroso (NO) nitro ($-NO_2$) and alkoxy (–OR) are always treated as substituent groups.

Ex. (i)



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

(ii)

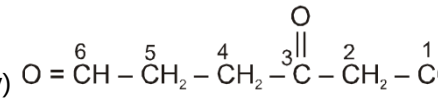


3-Oxobutan-1-oic acid [– COOH > – CO]

(iii)

4-Oxopentan-1-al [– CHO > C=O]

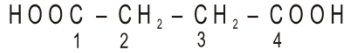
(iv)



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

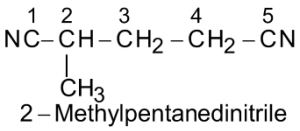
(3) If more than one same chain terminating group are present then the parent chain is selected including all principal functional groups (if possible) and numbring is done from that end which gives lowest locant to unsaturation and substituents.

Ex. (i)



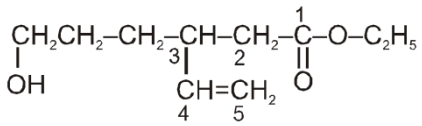
Butane-1, 4-dioic acid

(ii)



2 – Methylpentanedinitrile

(iii)

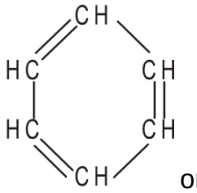


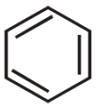
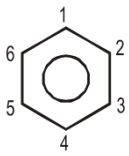
Ethyl 3-(3-hydoxy propyl) pent-4-enoate

Parent chain contains five rather than six carbon atoms.

Section (I) : IUPAC-Nomenclature of Aromatic compounds

The aromatic compounds are cyclic compounds which contain one or more benzene 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  or 

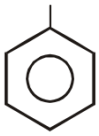
(i) Nuclear substituted :

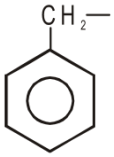
If the functional group is directly attached to the benzene ring then in the IUPAC system they are named as derivatives of benzene. The position of the substituents in disubstituted benzenes are indicated either by prefixes such as o-(ortho) for 1, 2, m-(meta) for 1, 3 and p-(para) for 1, 4 position.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

(ii) Side chain substituted :

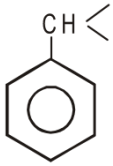
If the functional group is present in the side chain of the benzene ring then in the IUPAC system, these are usually named as phenyl derivatives of the corresponding aliphatic compounds.
The IUPAC and common names of a few important members of each family are given below.

Aryl groups :


Phenyl

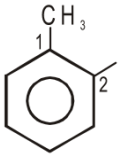


Benzyl

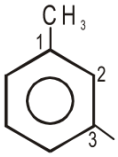


Benzal

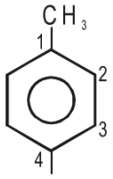
Benzo



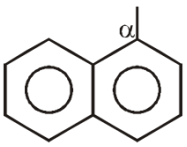
2 – Tolyl or (o – Tolyl)



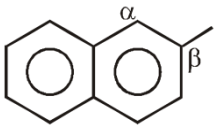
3 – Tolyl or (m – Tolyl)



4 – Tolyl or (p – Tolyl)

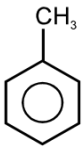


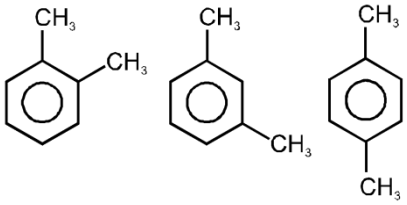
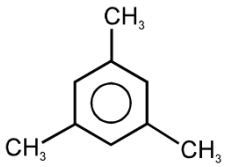
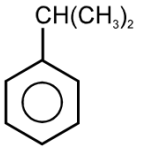
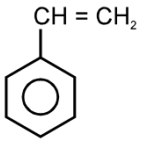
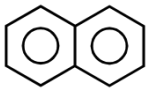
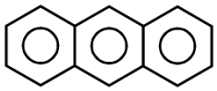
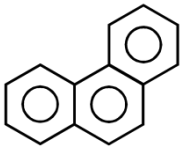
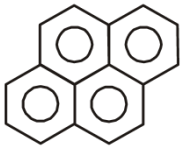
α-naphthyl



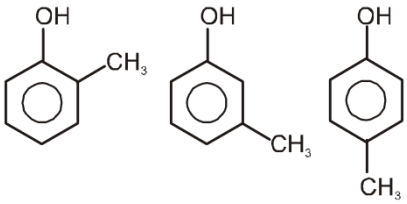
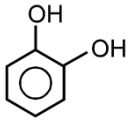
β-naphthyl

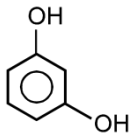
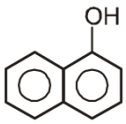
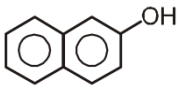
Other aromatic examples

S.No.	Compounds	Common Name	IUPAC Name
Aromatic Hydrocarbons :			
1.		Toluene	Methylbenzene or Toluene

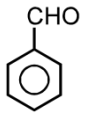
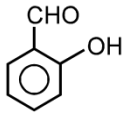
2.		Xylene (o,m,p)	(o,m,p) Dimethylbenzene
3.		Mesitylene	1, 3, 5 – Trimethyl benzene
4.		Cumene	Isopropylbenzene
5.		Styrene	Phenyl ethene or Ethenylbenzene
6.		Naphthalene	Naphthalene
7.		Anthracene	Anthracene
8.		Phenanthrene	Phenanthrene
9.		Pyrene	Pyrene

Aromatic Alcohols :

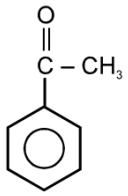
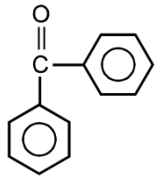
10.		Carbolic acid	Phenol
11.		(o, m, p) cresol	Methylphenol
12.		Catechol	Benzene-1,2-diol

13.		Resorcinol	Benzene-1,3-diol
14.		Hydroquinone	Benzene-1,4-diol
15.		α-Naphthol	Naphthalen-1-ol
16.		β-Naphthol	Naphthalen-2-ol

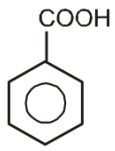
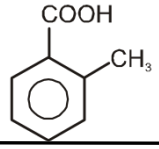
Aromatic Aldehydes :

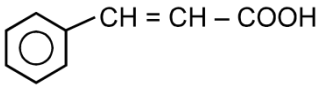
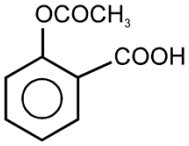
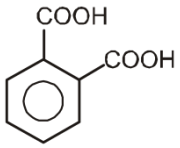
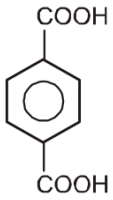
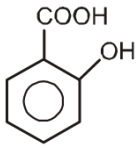
17.		Oil of bitter almonds	Benzenecarbaldehyde
18.		Salicylaldehyde	2 – Hydroxy benzaldehyde (2 – Hydrobenzene carbaldehyde)

Aromatic Ketones :

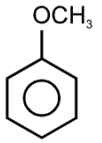
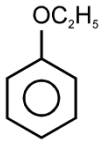
19.		Acetophenone	Acetophenone
20.		Benzophenone (Diphenylketone)	Bennzophenone

Aromatic Acids :

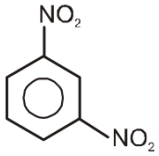
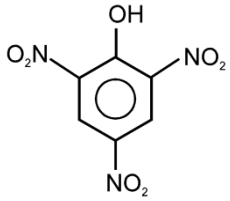
21.		Benzoic acid	Benzenecarboxylic acid (Benzoic acid)
22.		o-toluic acid	2 – Methylbenzene carboxylic acid

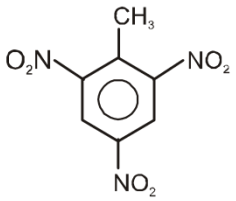
23.		Cinnamic acid	3–Phenylprop–2–enoic acid
24.		Aspirin (Acetyl salicylic acid)	2-Ethanoyloxybenzene carboxylic acid
25.		Phthalic acid	Benzene 1,2–dicarboxylic acid
26.		Terephthalic acid	Benzene 1,4–dicarboxylic acid
27.		Salicylic acid	2-Hydroxybenzene carboxylic acid

Aromatic Ether :

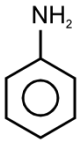
28.		Anisole	Methoxybenzene
29.		Phenetol	Ethoxybenzene

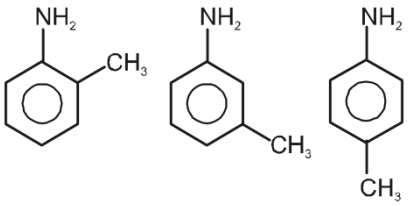
Aromatic Nitro Compounds :

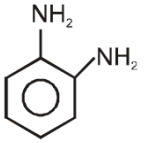
30.		Oil of mirbane	Nitrobenzene
31.		—	1,3 – Dinitrobenzene (m – Dinitrobenzene)
32.		Picric acid	2,4,6 –Trinitrophenol

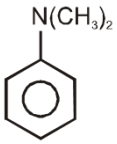
33.  — 2,4,6 – Trinitrotoluene(TNT) an explosive

Aromatic Amines :

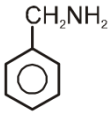
34.  Aniline Aniline (Benzenamine)

35.  (o, m, p) Toluidine Methylaniline

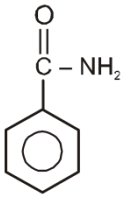
36.  o-Phenylenediamine Benzene-1,2-diamine

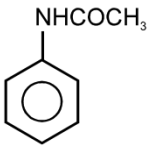
37.  N,N–Dimethylaniline N,N–Dimethylbenzenamine

Aromatic Alkyl Amines :

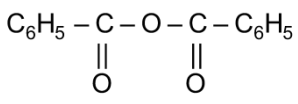
38.  Benzylamine Phenylmethanamine

Aromatic Amides :

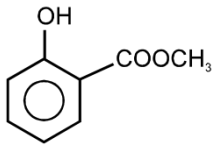
39.  Benzamide Benzenecarboxamide

40.  Acetanilide N-Phenylethanamide

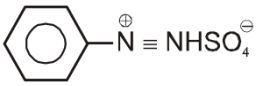
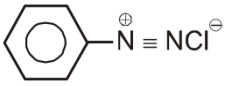
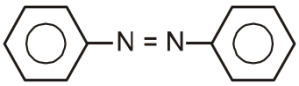
Aromatic Anhydrides :

41.  Benzoic anhydride Benzenecarboxylic anhydride

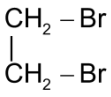
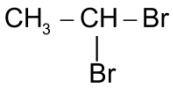
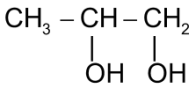
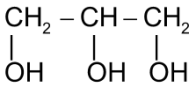
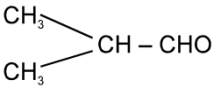
Aromatic Esters :

42.		Oil of winter green (Methyl salicylate)	Methyl 2 – hydroxy benzenecarboxylate

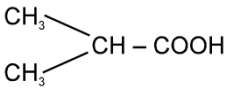
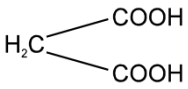
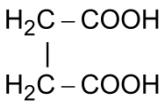
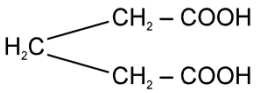
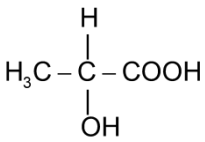
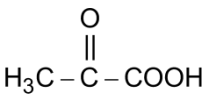
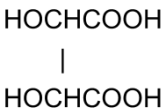
Arenediazonium Salts :

43.		—	Benzene diazonium hydrogen sulphate
44.		—	Benzene diazonium chloride
45.		—	Diazobenzene

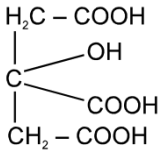
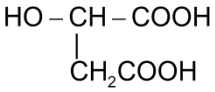
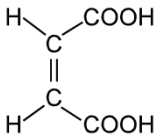
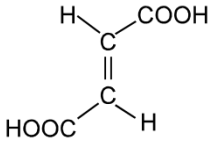
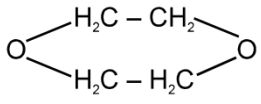
Common and IUPAC Names of Some Organic Compounds

S.No.	Compund	Common Names	IUPAC Name
1.		Ethylene dibromide	1,2-Dibromoethane
2.		Ethylidene bromide	1,1-Dibromoethane
3.	$CH \equiv C - CH_2 - OH$	Propargyl alcohol	Prop-2-yn-1-ol
4.		Propylene glycol	Propane-1, 2-diol
5.	$HO - CH_2 - CH_2 - CH_2 - OH$	Trimethylene glycol	Propane-1,3-diol
6.		Glycerol or Glycerine	Propane-1,2,3-triol
7.	$H - CHO$	Formaldehyde	Methanal
8.	$CH_3 - CHO$	Acetaldehyde	Ethanal
9.	$CH_3CH_2CH_2 - CHO$	n-Butyraldehyde	Butanal
10.		Isobutyraldehyde	2-Methylpropanal

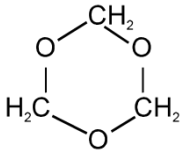
S.No.	Compound	Common Name	IUPAC Name
11.	$CH_2 = CH - CHO$	Acrolein	Propenal

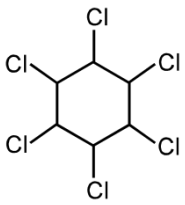
12.	$CH_3CH = CH - CHO$	Crotonaldehyde	But-2-enal
13.	$CH_3 - CO - CH_3$	Dimethyl ketone or Acetone	Propanone
14.	$CH_3 - CO - CH_2CH_3$	Ethyl methyl ketone	Butanone
15.	$CH_3 - CO - CH_2CH_2CH_3$	Methyl n-propyl ketone	Pentan-2-one
16.	$CH_3CH_2 - CO - CH_2CH_3$	Diethyl ketone	Pentan-3-one
17.	$CH_3CO - CH = CH_2$	Methylvinyl ketone	But-3-en-2-one
18.	$H - COOH$	Formic acid	Methanoic acid
19.	$CH_3 - COOH$	Acetic acid	Ethanoic acid
20.	$CH_3CH_2CH_2 - COOH$	n-Butyric acid	Butanoic acid
21.	$CH_3CH_2CH_2CH_2COOH$	n-Valeric acid	Pentanoic acid
22.		Iso-butyric acid	2-Methylpropanoic acid
23.	$CH_2 = CH - COOH$	Acrylic acid	Propenoic acid
24.		Oxalic acid	Ethanedioic acid
25.		Malonic acid	Propanedioic acid
26.		succinic acid	Butanedioic acid
27.		Glutaric acid	Pentanedioic acid
28.		Lactic acid	2-Hydroxypropanoic acid
29.		Pyruvic acid	2-Oxopropanoic acid
30.		Tartaric acid	2,3–Dihydroxybutane dioic acid

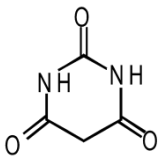
S.No.	Compound	Common Name	IUPAC Name

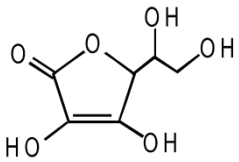
31.		Citric acid	2-Hydroxypropane-1-2,3-tricarboxylic acid
32.		Malic acid	2-Hydroxy-butanedioic acid
33.		Maleic acid	cis-But-2-enedioic acid
34.		Fumaric acid	trans-But-2-enedioic acid
35.	$CH_3 - N^+ \equiv C^-$	[Methyl isocyanide or Methyl carbyl amine]	Methane isocyanide
36.	$H_3C - CH = CH - COOH$	Crotonic acid	But-2-enoic acid
37.	$H - COOCH_3$	Methyl formate	Methyl methanoate
38.	$H - COOC_2H_5$	Ethyl formate	Ethyl methanoate
39.	$CH_3 - COOC_2H_5$	Ethyl acetate	Ethyl ethanoate
40.	H – COCl (unstable)	Formyl chloride	Methanoyl chloride
41.	$CH_3 - COCl$	Acetyl chloride	Ethanoyl chloride
42.	$(CH_3CO)_2O$	Acetic anhydride	Ethanoic anhydride
43.	$(CH_3CH_2CO)_2O$	Propionic anhydride	Propanoic anhydride
44.	$H - CONH_2$	Formamide	Methanamide
45.	$CH_3 - CONH_2$	Acetamide	Ethanamide
46.	$CH_3 - CH_2 - CONH_2$	Propionamide	Propanamide
47.	$CH_3 - O - N = O$	Methyl nitrite	Methyl nitrite
48.	$CH_3CH_2 - O - N = O$	Ethyl nitrite	Ethyl nitrite
49.	$H_2N - SO_3H$	Sulphamic acid	Aminosulphonic acid
50.	$CH_3 - CN$	Methyl cyanide or Acetonitrile	Ethanenitrile
51.		Dioxane	-1, 4-Dioxacyclohexane

S.No.	Compound	Common Name	IUPAC Name

52.  Trioxane 1,3,5-Trioxacyclohexane

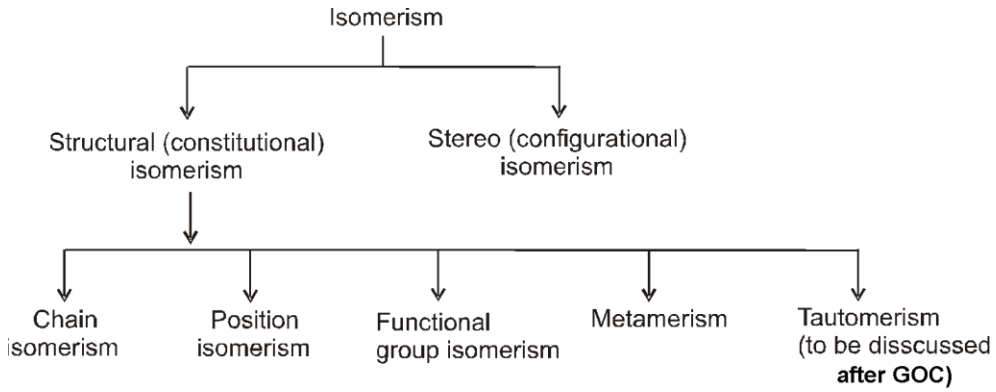
53.  (Gammexane or Lindane or 666) BHC [Benzene hexachloride] Hexachlorocyclohexane

54.  Barbituric acid

55.  Ascorbic acid

Structural Isomerism

Classification.



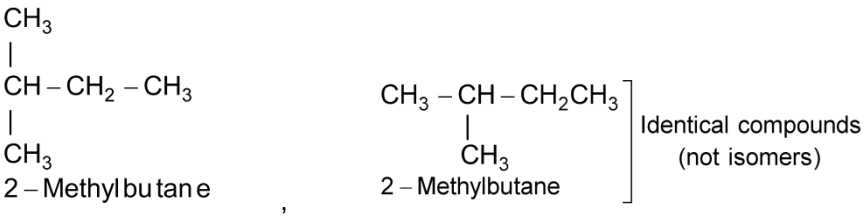
Section (J & K) : Structural Isomerism

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

Note : Structural isomers have always different IUPAC name

Ex-1. $\underset{\text{But}-2-\text{ene}}{CH_3-CH=CH-CH_3}$, $\underset{\text{But}-1-\text{ene}}{CH_3CH_2CH=CH_2}$] structural Isomers

Ex-2.



Isomers	Characteristics	Conditions
(1) Chain Isomers	They have different size of main chain or side chain	They should have same nature of locants
(2) Positional Isomers	They have different position of locants/multiple bond/functional group	They should have same size of main chain, side chain, nature of locants, multiple bonds and functional groups
(3) Functional Isomers	Different nature of functional group	Chain and positional isomerism is not considered
(4) Metamerism	Different nature of alkyl group along a polyvalent functional group	They should have same nature of functional groups. Chain & positional isomerism ignored
(5) Tautomerism	Different position of hydrogen atoms	The two functional isomers remains in dynamic equilibrium to each other

Ex-3. Relationship between the given compounds-

(a) (i) $CH_3 – CH_2–CH_2 – CH_3$

Butane

Size of main chain = 4

Size of side chain = 0

(ii) $CH_3 – \underset{\displaystyle CH_3}{\underset{|}{CH}} – CH_3$

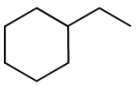
2–Methylpropane

Size of main chain = 3

Size of side chain = 1

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

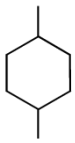
(b) (i) 1–Ethylcyclohexane



Size of main chain = 6

Size of side chain = 2

(ii) 1,4–Dimethylcyclohexane



Size of main chain = 6

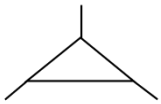
Size of side chain 1 = 1

Size of side chain 2 = 1

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

(c) (i) Cyclohexane

(ii) 1,2,3–Trimethylcyclopropane



Size of main chain = 6
Size of side chain = 0

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) $H_3C-CH_2-CH=CH_2$ (but – 1 – ene)
$H_3C-CH=CH-CH_3$ (but – 2 – ene)] position isomers

(e) $HC\equiv C-CH_2-CH_2-CH_3$ (pent – 1 – yne)
$H_3C-C\equiv C-CH_2-CH_3$ (pent – 2 – yne)] position isomers

(f) (i) CH_3-CH_2OH
Ethanol
Functional groups – OH

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

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

(g) (i) $CH_3-\overset{\overset{O}{\|}}{C}-OH$ Ethanoic acid

Functional groups – COOH

(ii) $H-\overset{\overset{O}{\|}}{C}-OCH_3$ Methyl methanoate

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

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

(h) (i) $C_2H_5-O-C_2H_5$
Diethyl ether
Hydrocarbon groups – C_2H_5 , – C_2H_5

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

Structure (i) & (ii) are metamers.

(i) (i) $CH_3-\overset{\overset{O}{\|}}{C}-CH_3$ (ketone)

(ii) $CH_2=\overset{\overset{OH}{|}}{C}-CH_3$ (enol)

Structure (i) & (ii) are tautomers.