Unit

1

Classification, Nomenclature, and Isomerism

I. ORGANIC COMPOUNDS

Organic compounds are chemical compounds comprises carbon atoms covalently linked to the other elements/atoms. They are classified as follows **(Fig. 1.1)**:

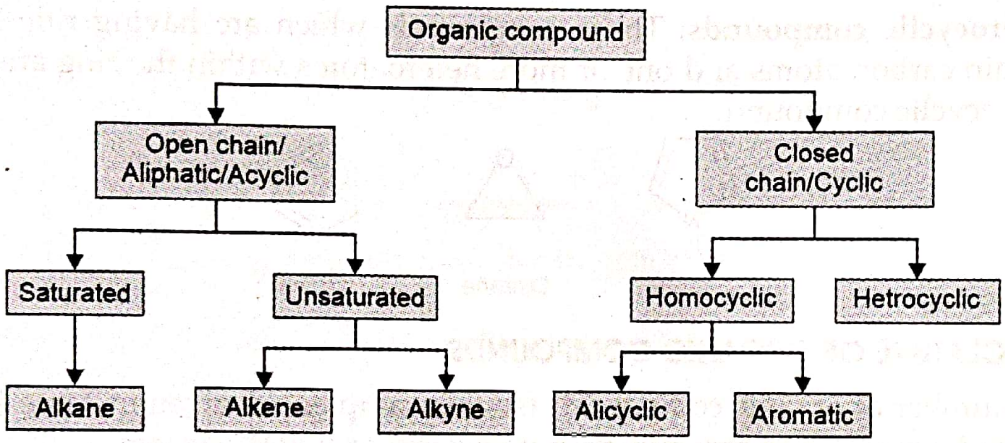
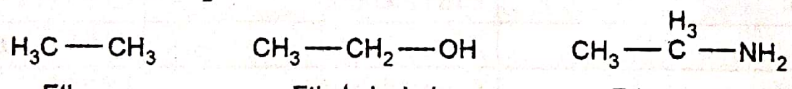


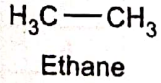
Fig. 1.1: Classification of organic compound (schematic)

1. **Alipathic compounds:** Compounds that contain open chain carbon atoms are called alipathic compounds. Examples:

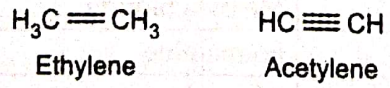


Alipathic compound can be saturated or unsaturated.

a. **Saturated compounds:** Compounds that contain carbon–carbon single bond are known as saturated compounds. Example: Ethane



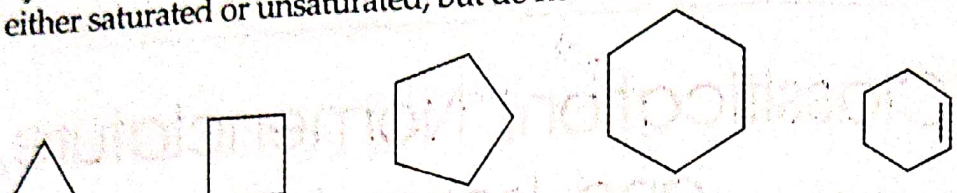
b. **Unsaturated compounds:** Compounds that contain carbon–carbon double or triple bonds are known as unsaturated compounds. Examples:



2. **Cyclic compounds:** Compounds that contain closed chain carbon atoms are called as cyclic compounds, they can be homocyclic and hetrocyclic.

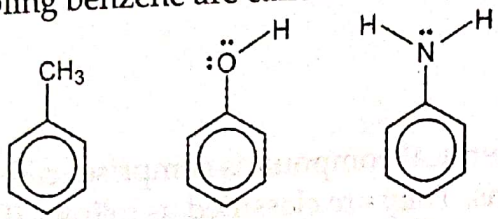
a. **Homocyclic compounds:** Compounds which are having ring structures, contain only carbon atom within the ring are known as homocyclic compounds. These are also known as carbocyclic compounds or carbocycles, and are further divided into two categories.

i. **Alicyclic compounds:** Compounds that contain one or more-carbon rings which may be either saturated or unsaturated, but do not have aromatic characters. Examples:



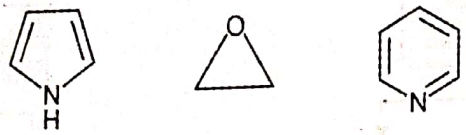
Cyclopropane Cyclobutane Cyclopentane Cyclohexane Cyclohexene

ii. **Aromatic compounds:** The compounds that have structures and chemical properties resembling benzene are called aromatic compounds. Examples;



Toluene Phenol Aniline

b. **Heterocyclic compounds:** Those compounds which are having ring structures, contain carbon atoms and one or more heteroatoms within the ring are known as heterocyclic compound.



Pyrrole Oxirane Pyridine

II. NOMENCLATURE OF ORGANIC COMPOUNDS

There are number of organic compounds (some examples are given in Table 1.1), which can be named according to common naming system or IUPAC system.

Table 1.1: Some examples of organic compounds

S. No.	Class of compounds	Example	Chemical formula
1	Alcohol	Ethyl alcohol	CH_3CH_2OH
2	Ether	Diethyl ether	$CH_3CH_2OCH_2CH_3$
3	Aldehyde	Formaldehyde	HCHO
4	Ketone	Acetone	CH_3OCH_3
5	Carboxylic acid	Acetic acid	CH_3COOH
6	Ester	Methyl acetate	CH_3COOCH_3
7	Amine	Ethyl amine	$CH_3CH_2NH_2$
8	Nitro	Nitro methane	CH_3NO_2
9	Alkyl halide	Methyl chloride	CH_3Cl
10	Amide	Formamide	$CHONH_2$
11	Thiol	Ethanethiol	CH_3CH_2SH

A. Common System of Nomenclature

(A-1) Common System of Nomenclature for Alkanes

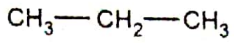
1. The first four members of series are called by their common name, i.e. methane, ethane, propane, butane, and higher alkanes are derived from Greek prefixes that indicate the number of carbon atoms in the molecule.

Examples:

(a) **Pentane:** Five number of carbons in its structure

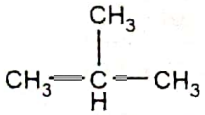
(b) **Hexane:** Six number of carbons in its structure and so on.

2. The prefix *n-* is used for those alkanes in which all carbons are in one continuous chain.



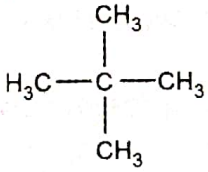
n-Propane

3. Prefix *iso-* is used for those alkanes which have a methyl group attached to second last carbon atom of a continuous chain.



iso-Butane

4. Prefix *neo-* is used for those alkanes which have two methyl groups attached to second last carbon atom of a continuous chain.



neo-Pentane

5. Alkyl group is formed by removing one hydrogen from an alkane, the suffix of this group is -yl.
6. Non-alkyl groups are F: Fluro, Cl: Chloro, Br: Bromo, I: Iodo, NO_2: Nitro, NH_2: Amino, and OH: Hydroxy.

B. IUPAC System of Nomenclature

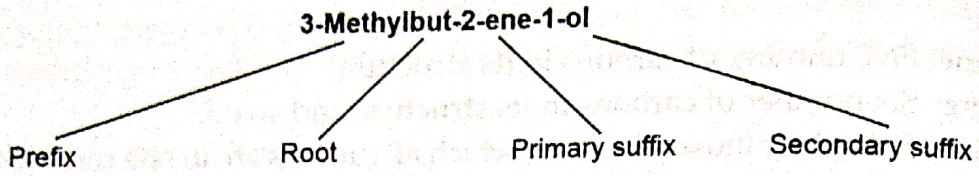
IUPAC stand for International Union of Pure and Applied Chemistry

General rules for IUPAC Nomenclature

1. Find the **longest continuous carbon** chain to considered as the parent chain
2. Determine the **root name** for this parent chain, one need to learn from Table 1.2.

Table 1.2: Root names depending upon number of carbon atom present in chain

No of "C" atom	Root name
1	Meth
2	Eth
3	Prop
4	But
5	Pent
6	Hext
7	Hept
8	Oct
9	Non
10	De



One of the examples of root name with prefix, primary suffix, and secondary suffix is given above.

3. Primary suffix indicates the nature of the carbon atom present in the chain.

Carbon chain	Primary suffix
Single bond between C atoms	**ane**
Double bond between C atoms	**ene**
Triple bond between C atoms	**yne**

4. If the parent chain contains two, three or more double or triple bonds, then the numerical prefixes such as di (for two), tri (for three), tetra (for four), etc. are added to the primary suffix.
5. If both double and triple bonds are present between the C atoms 'ene' comes before, 'yne', for example

$$HC{\equiv}C{-}CH_2CH_2{-}CH{=}CH_2$$

Hex-1-en-5-yne

6. **Secondary suffix** defines the **family** or **functional group** in the organic compound. Functional group is the reactive part of an organic compound. The various functional groups with their corresponding suffixes are given in Table 1.3.

Table 1.3: Functional groups with their corresponding suffixes

Functional group	Class of compound	Suffix
–COOH–	Carboxylic acids	-oic acid
–COOR–	Ester	-oate
–COX (X=F, Cl, Br, I)	Acyl halides	-oyl halide
$–CONH_2–$	Acid amide	-amide
–CN–	Nitriles	-nitrile
–CHO–	Aldehyde	-al
>C=O–	Ketones	-one
–OH–	Alcohol	-ol
$–NH_2–$	Amine	-amine
–C=C–	Alkene	-ene
–C≡C–	Alkyne	-yne

7. **Prefix** indicates the element which is fixed or attached before or at the beginning. Hence a prefix is written before the root word.
prefix *Cyclo* is used for cyclic compounds only.
Certain groups in organic chemistry are written as prefixes. They are regarded as substituents, their prefixes are given in Table 1.4.

Table 1.4: Various substituents with their corresponding prefixes used for nomenclature

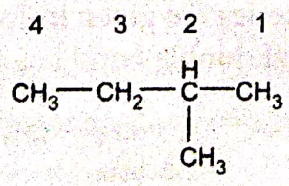
S. No.	Substituent	Prefix
1	–F	Fluoro-
2	–Cl	Chloro-
3	–Br	Bromo-
4	–I	Iodo-
5	$-NO_2$	Nitro-
6	–NO	Nitroso-
7	–N-N-	Diazo-
8	$-OCH_3$	Methoxy
9	$-OC_2H_5$	Ethoxy
10	–OH	Hydroxy
11	$-NH_2$	Amino
12	–COOH	Carboxy
13	$-SO_3H$	Sulpho
14	–COOR	Alkoxycarbon
15	–COCl	Haloformyl
16	$-CONH_2$	Carbamoyl
17	–CN	Cyano
18	–CHO	Formyl
19	>C=O	Keto/oxo
20	–SH	Mercapto

8. If the first substituents from either side have the same number, then the second substituent has the smaller number.
9. Determine the position, number and name of each substituent.
10. Number the chain in the direction such that position, number of first substituent is the small number.

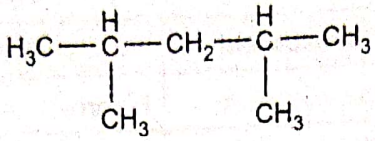
(B-1) IUPAC Rules for the Nomenclature of Alkanes (General formula C_nH_{2n+2})

General rules mentioned in point 1, 2, 3, 4, 5, 6, 7, 8 and 9 will be applicable for alkanes too, apart from these below mentioned rules are also applied for the nomenclature of alkanes. Various members of the series are given in Table 1.5.

1. Number the chain in the direction such that position, number of first substituent is the smallest number.

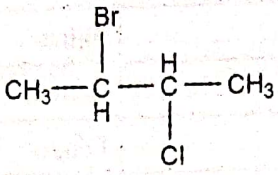


2. Indicate the number of identical groups by the prefixes di-, tri-, tetra-, etc.



2,4-Dimethylpentane

3. Place the position numbers and names of the substituent groups, in alphabetical order, before the root name.



2-Bromo-3-chlorobutane

4. The alkyl group is named by substituting the suffix 'ane' of the name of the corresponding alkane by 'yl', for e.g: CH_4–Methane becomes CH_3–Methyl.

Table 1.5: Various members of alkane series

Condensed structural formula	IUPAC name	Common name
CH_4	Methane	Methane
CH_3CH_3	Ethane	Ethane
$CH_3CH_2CH_3$	Propane	Propane
$CH_3CH_2CH_2CH_3$	Butane	*n*-Butane
$CH_3(CH_2)_3CH_3$	Pentane	*n*-Pentane
$CH_3(CH_2)_4CH_3$	Hexane	*n*-Hexane
$CH_3(CH_2)_5CH_3$	Heptane	*n*-Heptane
$CH_3(CH_2)_6CH_3$	Octane	*n*-Octane
$CH_3(CH_2)_7CH_3$	Nonane	*n*-Nonane
$CH_3(CH_2)_8CH_3$	Decane	*n*-Decane

(A-2) Common System of Nomenclature for Alkenes

1. The common names of the first four members named by changing **-ane to -ylene or ene.**
2. The Greek letters are used to distinguish isomers having double bond at the first and second carbon of the chain.

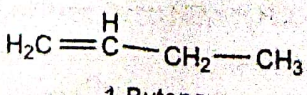
α-Butylene
1-Butene

β-Butylene
2-Butene

(B-2) IUPAC Nomenclature for Alkenes (General formula C_nH_{2n})

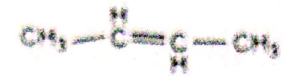
General rules mentioned in **point 1, 2, 3, 4, 5, 6, 7, 8** and **9** will be applicable for alkenes too, apart from these, below mentioned rules are also applied for the nomenclature of alkenes. Various members of the series are given in Table 1.6.

1. Number the longest chain so that double bond has the lowest possible number.



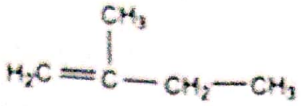
1-Butene

2. To indicate the position of C=C, add the number in front of alkene name.



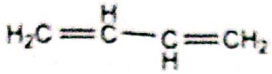
2-Butene

3. Side chain and substituents are named as usual and their position is indicated by number to show to which carbon atom they are attached.



2-Methy 1-1-butene

4. When there are two or three double bonds in a molecule di- and tri- will be added in name.



1,3-Butadiene

(A-3) Common System of Nomenclature for Alkynes

1. Acetylene is the common name for the first member of alkyne series.

Acetylene

2. Higher alkynes are regarded as alkyl derivatives of acetylene.

Dimethylacetylene

Table 1.6: Various members of alkene series

Condensed Structural Formula	IUPAC name
$CH_2=CH_2$	Ethene
$CH_2=CHCH_3$	Propene
$CH_2=CHCH_2CH_3$	1-Butene
$CH_2=CH(CH_2)_2CH_3$	1-Pentene
$CH_2=CH(CH_2)_3CH_3$	1-Hexene
$CH_2=CH(CH_2)_4CH_3$	1-Heptene
$CH_2=CH(CH_2)_5CH_3$	1-Octene
$CH_2=CH(CH_2)_6CH_3$	1-Nonene
$CH_2=CH(CH_2)_7CH_3$	1-Decene

(B-3) IUPAC Nomenclature for Alkynes (General formula: C_nH_{2n-2})

All rules mentioned for alkenes series is applicable for alkynes series also. Various members of the series are given in Table 1.7.

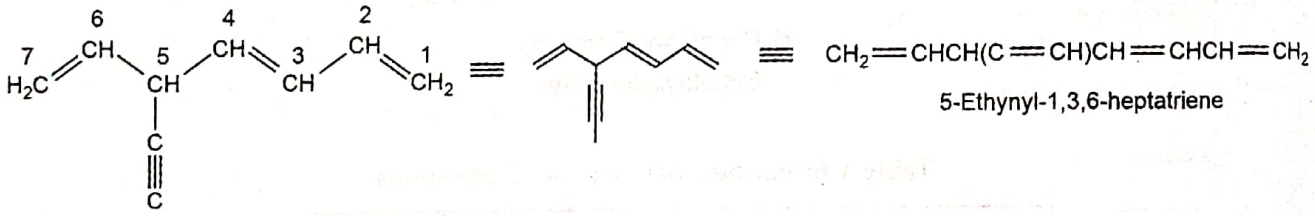
Table 1.7: Various members of alkyne series

Condensed Structural Formula	IUPAC name
$C{\equiv}CH$	Ethyne
$C{\equiv}CH\ CH_3$	Propyne
$C{\equiv}CHCH_2CH_3$	1-Butyne
$C{\equiv}CH(CH_2)_2CH_3$	1-Pentyne
$C{\equiv}CH(CH_2)_3CH_3$	1-Hexyne
$C{\equiv}CH(CH_2)_4CH_3$	1-Heptyne
$C{\equiv}CH(CH_2)_5CH_3$	1-Octyne
$C{\equiv}CH(CH_2)_6CH_3$	1-Nonyne
$C{\equiv}CH(CH_2)_7CH_3$	1-Decyne

Notes

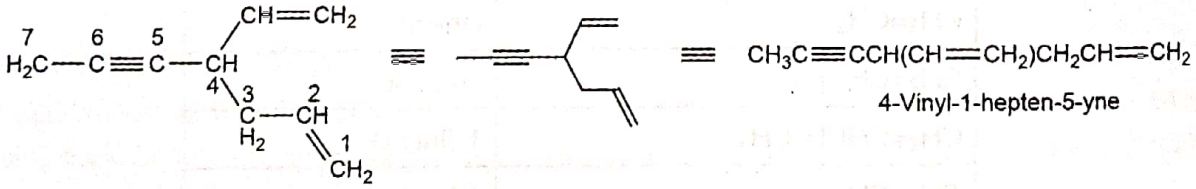
The root chain contains the maximum number of multiple bonds.

- If more than one such chain is found, the longest is choosen as the root.
- If the chains have equal length, the one with the most double bond is choosen (examples are given below).



$CH_2{=}CHCH(C{=}CH)CH{=}CHCH{=}CH_2$

5-Ethynyl-1,3,6-heptatriene

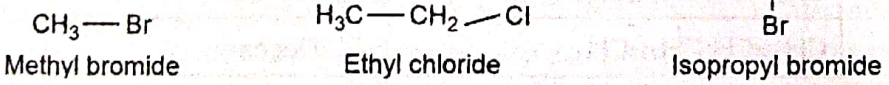


$CH_3C{\equiv}CCH(CH{=}CH_2)CH_2CH{=}CH_2$

4-Vinyl-1-hepten-5-yne

(A-4) Common System of Nomenclature for Alkyl Halides

1. Alkyl group attached to halogen atom is named first



$CH_3{-}Br$ Methyl bromide

$H_3C{-}CH_2{-}Cl$ Ethyl chloride

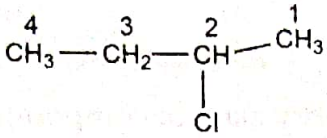
$(CH_3)_2CHBr$ Isopropyl bromide

(B-4) IUPAC Nomenclature for Alkyl Halide (General formula: $C_nH_{2n+1}X$ or RX)

Apart from general rules of IUPAC, other rules are mentioned below for alkyl halides.

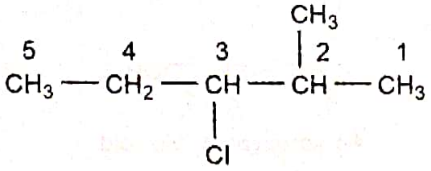
1. They are named as halogen substituted alkanes, i.e. haloalkanes (X = F, Cl, Br, I).

2. If the parent chain has no branching alkyl group, the position of halogen number is given by the number that corresponds to the carbon atom to which it is attached. The carbon atom bearing the halogen atom will bear the lowest number.



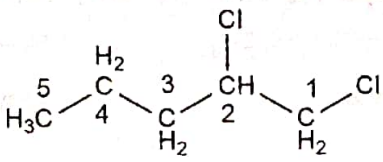
2-Chlorobutane

3. If the parent chain has branching alkyl group, number the chain from the end near to the first substituent.



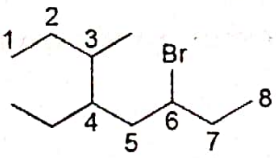
3-Chloro 2-methylpentane

4. If the compound contains two or more same halogen atoms of the same type they are named as **di-**, **tri-**, etc.

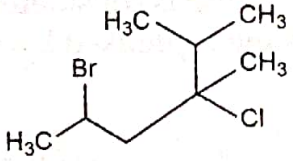


1,2-Dichloropentane

5. If the compound contains two or more different halogen/substituent atoms they are numbered according to their position on the chain but the name should be written in alphabetical order.



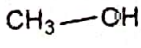
6-Bromo-4-ethyl-3-methyloctane



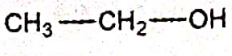
2-Bromo-4-chloro-4-isopropylpentane

(A-5) Common System of Nomenclature for Alcohol

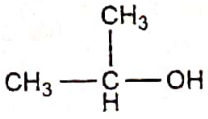
1. Here alcohol (R-OH) is named as alkyl alcohol.



Methyl alcohol



Ethyl alcohol



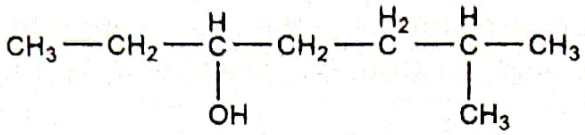
Iso-propyl alcohol

(B-5) IUPAC Nomenclature for Alcohol (General formula: C_nH_{2n+OH} or ROH)

Apart from general rules of IUPAC, other rules which are applicable for naming of alcohols are mentioned below.

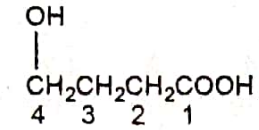
1. These are derived by replacing one hydrogen atom from an alkane by one hydroxyl group and in IUPAC system, these are called as *alkanols*. Their names have been derived by changing **-e** of corresponding alkane by **-ol** (suffix).
2. Number the chain so that carbon atom carrying the -OH group get the lowest number, position of -OH group is indicated by its number.

3. Indicate the position of other substituents or multiple bonds by numbers.



6-Methylheptan-3-ol

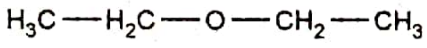
4. When OH is part of higher priority class of compound, it is named as hydroxy.
   Priority of functional groups:
   Acid > esters > aldehyde > ketone > alcohol > amine > alkene > alkyene > alkane > ethers > halides.



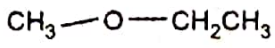
4-Hydroxybutanoic acid

(A-6) Common System of Nomenclature for Ethers

1. The two alkyl groups attached to oxygen named in alphabetical order and word *ether* is added. If the two alkyl groups are same (R-O-R), the prefix di- is used.



Diethyl ether

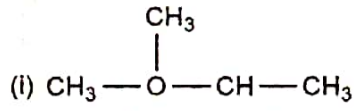


Ethylmethyl ether

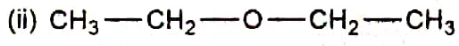
(B-6) IUPAC Nomenclature for Ethers (General formula: $C_nH_{2n+1}OC_nH_{2n+1}$ or -ROR¹)

Apart from general rules of IUPAC, other rules which are applicable for naming of ethers are mentioned below.

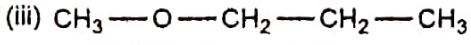
1. These are derived from alkanes by replacing one hydrogen atom by alkoxy group.
2. The larger alkyl group is considered to be alkanes or parent.
3. The name of alkane is prefixed by the name of alkoxy group and position number.



(i) 2-Methoxy propane



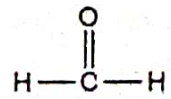
(ii) Ethoxy ethane



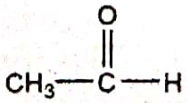
(iii) 1-Methoxy propane

(A-7) Common System of Nomenclature for Aldehyde

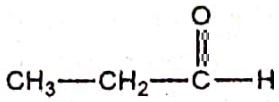
1. The name of simple aldehydes are derived from the common name of carboxylic acids.
2. The characteristic -ic acid ending in the common name of carboxylic acid is dropped and replaced by aldehyde.
   For example, 1C carboxylic acid is formic acid, so the name of corresponding aldehyde is formaldehyde and so on.



Formaldehyde



Acetaldehyde

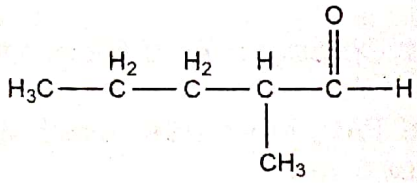


Propionaldehyde

(B-7) IUPAC Nomenclature for Aldehyde (General formula: $C_nH_{2n+1}CHO$ or -RCHO)

Apart from general rules of IUPAC, other rules which are applicable for naming of aldehydes are mentioned below.

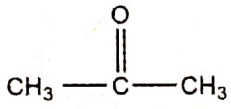
1. These compounds are obtained by replacing a hydrogen atom attached to the terminal carbon atom in alkane molecule by an aldehyde (CHO) group. These are called *alkanals*.
2. The names of individual members are derived by changing **-e** of corresponding alkane by **-al**.
3. The numbering of longest continuous chain starts with C-1 as the carbon bearing the aldehyde group.
4. The substituents are indicated by name and position number.



2-Ethylpentanal

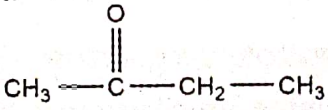
(A-8) Common System of Nomenclature for Ketone

1. The members of these series are known as dialkyl ketones, first member, however is popular as acetone.



Acetone

2. For unsymmetrical ketones naming of alkyl groups are done in alphabetical order, adding the word ketone at last.

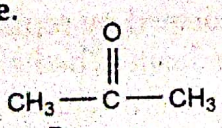


Ethyl-methyl ketone

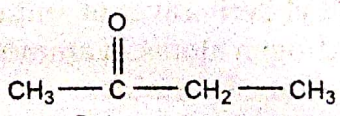
(B-8) IUPAC Nomenclature for Ketone (General Formula: $C_nH_{2n+1}COC_nH_{2n+1}$ or -RCOR')

Apart from general rules of IUPAC, other rules which are applicable for naming of ketones are mentioned below.

1. These are obtained by replacing two hydrogen atoms attached to the non-terminal carbon atom in alkane molecule by a divalent oxygen atom. They are known as alkanones.
2. The names of individual members are derived by replacing **-e** of the corresponding alkane by **-one**.

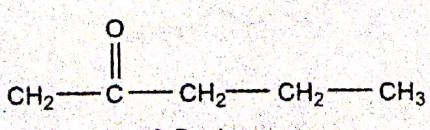


Propanone



Butanone

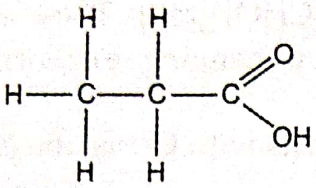
3. For naming higher ketones, it becomes necessary to assign a positional number to the carbonyl group.



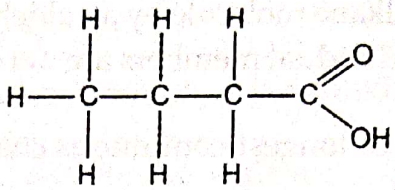
2-Pentanone

(A-9) Common System of Nomenclature for Carboxylic Acid

1. The longest carbon chain containing carboxylic group is selected and the carboxylic acid is named by replacing **-e** of the corresponding alkane by **-ic** acid as given in below examples.



Propionic acid

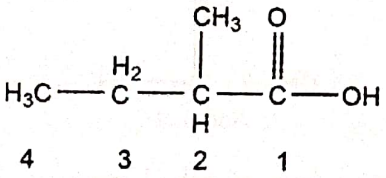


Butyric acid

(B-9) IUPAC Nomenclature for Carboxylic Acid (General formula: $C_nH_{2n+1}COOH$ or –RCOOH)

Apart from general rules of IUPAC, other rules which are applicable for naming of carboxylic groups are mentioned below.

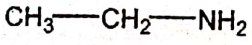
1. One hydrogen atom in alkane molecule is replaced by a carboxyl (COOH) group.
2. The longest carbon chain containing carboxylic group is selected and they are named by replacing the terminal **-e** of the corresponding alkane by **-oic** acid.
3. The selected carbon chain is numbered 1, 2, 3, 4, etc. to indicate the position of the side chains attached to it.



2-Methyl butanoic acid

(A-10) Common System of Nomenclature for Amine

1. The longest carbon chain containing amine group is selected and the carboxylic acid is named by replacing the **-e** of the corresponding alkane by **-alkylamine**.

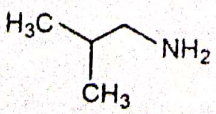


Ethyl amine

(B-10) IUPAC Nomenclature of Amine (General formula: $C_nH_{2n+1}NH_2$ or $-RNH_2$)

Apart from general rules of IUPAC, other rules which are applicable for naming of amines are mentioned below.

1. These are the alkyl derivatives of ammonia. They are formed by replacing one, two or all the three hydrogen atoms in ammonia with alkyl radicals. The name is derived by replacing **-e** of alkane by **amine**.
2. The longest carbon chain containing amine group is selected. The selected carbon chain is numbered 1, 2, 3, 4, etc. to indicate the position of the side chains attached to it.

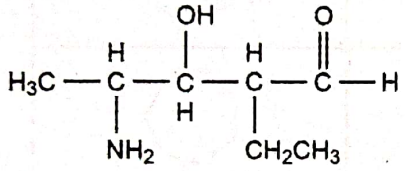


2-Methylpropan-1-amine

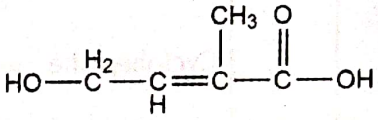
(B-11) IUPAC Nomenclature of Amine for Polyfunctional Group

Polyfunctional group means when one compound contains more than one functional group and/or substituent and/or multiple bond.

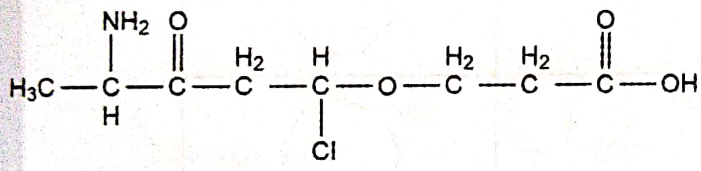
1. The group of **highest priority** is indicated by **suffix**, the others **substituents** are indicated by **prefix**, as per given priority of functional group:
   Carboxylic acid > sulphonic acid > anhydride > ester > acid chloride > acid amide > nitrile > aldehyde > ketone > alcohol > amines > alkene > alkyne > ether > alkyl halide > nitro amine
2. Find the highest priority functional group. Determine and name the longest continuous carbon chain that includes this group. It will be considered as parent chain.
3. Place the prefixes, with appropriate position numbers, in alphabetical order before the root name.
4. Suffix and prefix for each functional group, given in Tables 1.3 and 1.4 respectively.



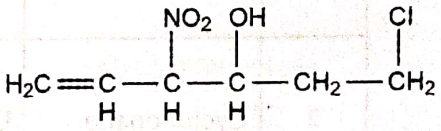
4-Amino-2-ethyl-3-hydroxypentanal



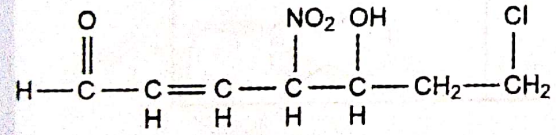
4-Hydroxy-2-methylbut-3-enoic acid



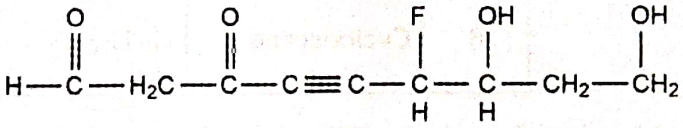
3-(4-Amino-1-chloro-3-oxopentyloxy) propanoic acid



1-Chloro-4-nitrohex-5-en-3-ol



7-Chloro-5-hydroxy-4-nitrohept-2-enal



6-Fluoro-7,9-dihydroxy-3-oxonon-4-enoic acid

Nomenclature of Carbocyclic Compounds

A cyclic organic compound containing all carbon atoms in ring formation is designated as a carbocyclic/homocyclic compounds. As in classification section, it is given that carbocyclic compounds are further classified as alicyclic and aromatic compounds.

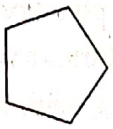
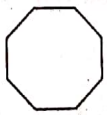
Nomenclature of Alicyclic compounds

All the rules are same for cycloalkanes, cycloalkene and cycloalkyne as discussed for alkane, alkene and alkyne, respectively.

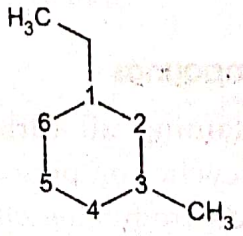
Summary

1. *Determine the parent chain:* The parent chain contains the most carbon atoms. Some examples are given in Table 1.8.

Table 1.8: Nomenclature of alicyclic compounds with some example

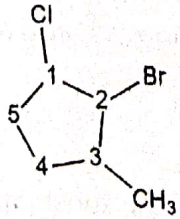
S. No.	Cycloalkane	Molecular Formula	Basic Structure
1	Cyclopropane	C_3H_6	
2	Cyclobutane	C_4H_8	
3	Cyclopentane	C_5H_{10}	
4	Cyclohexane	C_6H_{12}	
5	Cycloheptane	C_7H_{14}	
6	Cyclooctane	C_8H_{16}	
7	Cyclononane	C_9H_{18}	
8	Cyclodecane	$C_{10}H_{20}$	

2. Number the substituents of the chain so that the sum of the numbers is the lowest poss

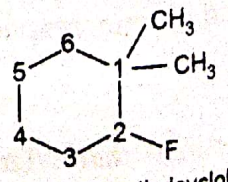


1-Ethyl-3-methylcyclohexane

3. Name the substituents and place them in alphabetical order.

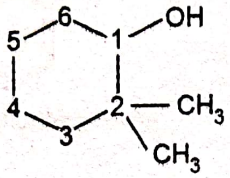


2-Bromo-1-chloro-3-methylcyclopentane

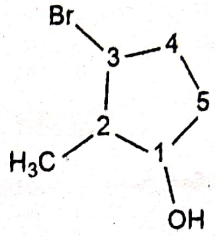


2-Fluoro-1,1,-dimethylcyclohexane

4. Cyclic hydrocarbons have the prefix "cyclo-" and have an "-alkane" ending unless there is an alcohol substituent present. When an alcohol substituent is present, the molecule has an "-ol" ending.

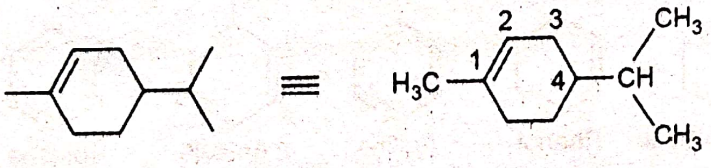


2,2-Dimethylcyclohexanol

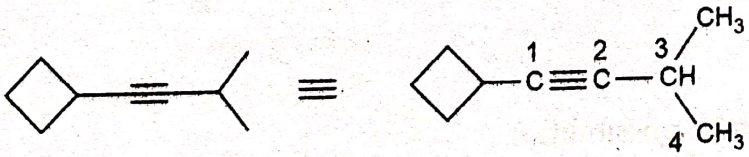


3-Bromo-2-methylcyclopentanol

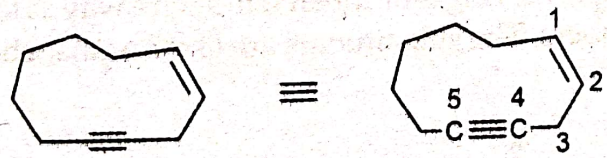
5. The root chain must be numbered from the end nearest a double bond carbon atom



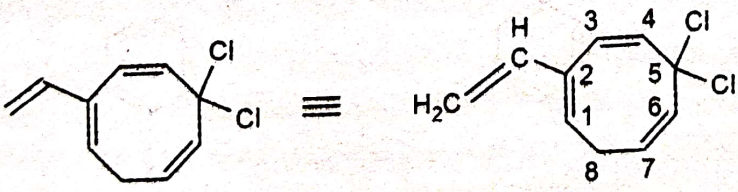
4-Isopropyl-1-methylcyclohexene



1-Cyclobutyl-3-methyl-1-butyne



1-Cyclodecen-4-yne

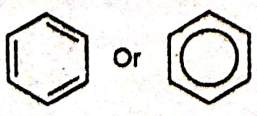


5,5-Dichloro-2-vinyl-1,3,6-cyclooctatriene

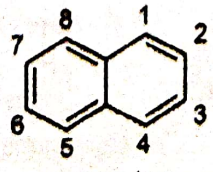
Nomenclature of Aromatic Compounds: Aromatic compounds are derived from benzene and similar ring systems.

As with aliphatic nomenclature described above—Determining the root name of the parent ring; determining priority, name, and position number of substituents; and assembling the name in alphabetical order, functional group priorities are the same in aliphatic and aromatic nomenclature.

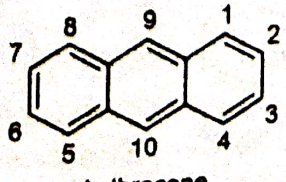
A. Common Parent Ring Systems



Benzene



Naphthalene



Anthracene