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PHARMACEUTICAL ORGANIC CHEMISTRY – I

UNIT 1

TOPIC :

- **Classification, nomenclature and isomerism**

  Classification of Organic Compounds

  Common and IUPAC systems of nomenclature of organic compounds

  (up to 10 Carbons open chain and carbocyclic compounds)

  Structural isomerisms in organic compounds

Introduction to Organic Chemistry

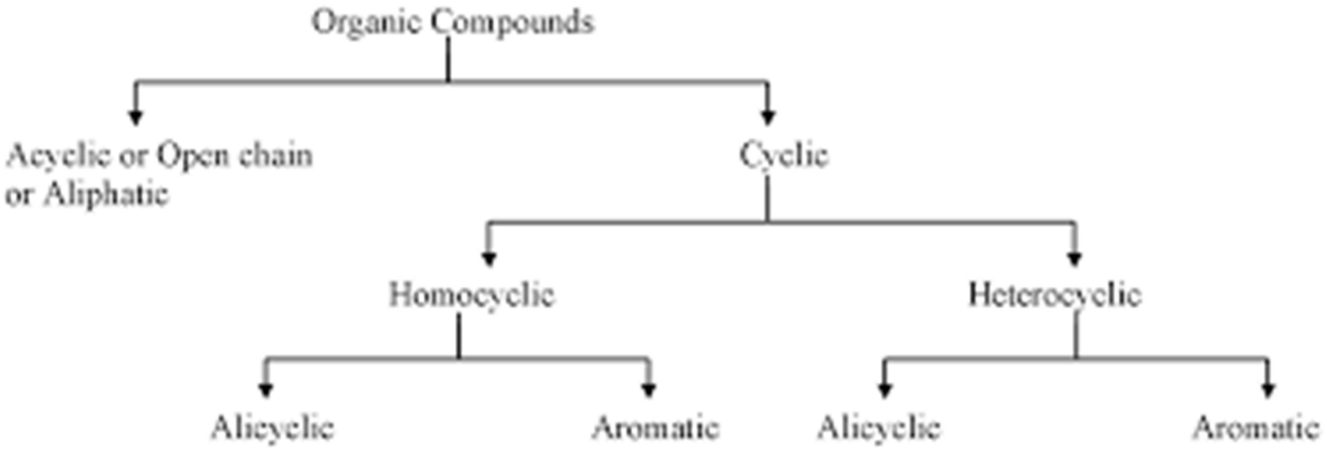
→ Organic chemistry is the branch of chemistry that deals with the structure, properties, composition, reactions, and synthesis of compounds containing carbon.

→ These compounds are called organic compounds, and they are primarily made of carbon and hydrogen, often with oxygen, nitrogen, sulfur, phosphorus, and halogens.

ORGANIC COMPOUNDS

- **Organic compounds** are chemical compounds that contain **carbon atoms** bonded **mainly with hydrogen**, and sometimes with **oxygen, nitrogen, sulfur, phosphorus, or halogens**. These compounds are the basis of all life and are studied under **organic chemistry**.
- Example : CH_4, C_2H_6, etc

Classification of Organic Compounds



Acyclic compounds (open chain compounds)

→ In these compounds, carbon atoms are arranged in the form of open chains.
→ The chains may be straight or branched but do not form a ring structure.
→ The terminal carbon atoms are free and are not connected to each other.
→ Initially, these compounds were called aliphatic compounds because they were derived from animal or vegetable fats.

Classification of Acyclic / Open-Chain Organic Compounds

1. Saturated Acyclic Compounds (Alkanes)
    - These compounds contain only single bonds (C–C and C–H).
    - They are also known as paraffins.
    - They follow the general formula: C_nH_{2n+2}
    - They are less reactive and undergo substitution reactions.

Examples:

- Methane (CH_4)
- Ethane (C_2H_6)
- Propane (C_3H_8)

2. Unsaturated Acyclic Compounds
    - ➢ These compounds contain one or more multiple bonds (double or triple bonds) between carbon atoms. They are more reactive than saturated compounds and usually undergo addition reactions.
    - ➢ They are further classified into:

a. *Alkenes* ***(With double bonds)***

- Contain at least one **C=C double bond**

- General formula: $\mathbf{C_nH_{2n}}$

Examples:

- Ethene (C_2H_4)
- Propene (C_3H_6)

b. *Alkynes* ***(With triple bonds)***

- Contain at least one **C≡C triple bond**
- General formula: $\mathbf{C_nH_{2n-2}}$

Examples:

- Ethyne (C_2H_2)
- Propyne (C_3H_4)

Cyclic / Closed-Chain Organic Compounds

- Cyclic or closed-chain organic compounds are compounds in which one or more chains of atoms form a ring (closed loop) in the molecule.
- In these compounds, the terminal carbon atoms are linked to each other, forming a closed ring structure.
- The ring may contain only carbon atoms (homocyclic) or carbon along with other atoms like oxygen, nitrogen, or sulfur (heterocyclic).

Classification of Cyclic Compounds:

→ Cyclic compounds are broadly classified into two types:

1. Homocyclic Compounds
   - (Ring made up of only carbon atoms)
   - These are further divided into:

a. *Alicyclic Compounds*

- Non-aromatic (do not follow aromatic rules)

- Have closed-ring structures of carbon atoms
- Can be saturated or unsaturated
- Examples: Cyclopropane, Cyclobutane, Cyclohexene

b. *Aromatic Compounds*

- Contain benzene rings or similar structures
- Are highly stable due to resonance
- Follow Hückel's Rule ($4n + 2\ \pi$ electrons)
- Examples: Benzene, Toluene, Naphthalene

2. Heterocyclic Compounds

➢ (Ring contains carbon + other atoms like N, O, S)

➢ Important in biological molecules and drugs

Examples :

- Furan (contains oxygen)
- Pyridine (contains nitrogen)
- Thiophene (contains sulfur)

Nomenclature Of Organic Compounds

There are two system of naming of organic compounds

1. Common or Trivial system
2. IUPAC System

Common System of Nomenclature of Organic Compounds:

→ According to this system, Organic compounds were named after the source from which they were first isolated

For example :

→ Urea got its name since the compound was first obtained from the urine of mammals.

→ Methyl alcohol was called wood spirit since it could be obtained by the destructive distillation of wood.

→ Acetic Acid got its name from the acetum since it is present in vinegar.

→ Formic acid was derived from formicus since it could be obtained by the destructive distillation of red ants.

→ Citric acid is named so because it is found in citrus fruits..

Drawbacks of the Common or Trivial Nomenclature System

- Several trivial names can exist for one specific compound. An example of this can be observed in the alternate names of Phenol, for which names such as hydroxybenzene and carbolic acid also exist.
- The Trivial nomenclature system is limited to only a few compounds in each specific group. An example of this is: the first two members belonging to the carboxylic acid group have the trivial names of formic acid and acetic acid. However, no trivial names exist for carboxylic acids with a greater number of atoms.
- There exist no particular set of guidelines for the nomenclature of complex compounds in the trivial system

IUPAC Nomenclature

→ IUPAC stands for International Union of Pure and Applied Chemistry.

→ The purpose of the IUPAC system of nomenclature is to establish a universal and standardized method for naming organic compounds.

→ This helps in clear communication of chemical names worldwide.

→ The IUPAC name of any organic compound essentially consists of five parts, i.e.

- Word root
- Primary Suffix
- Secondary Suffix
- Primary Prefix
- Secondary Prefix

Structure of IUPAC Name

Secondary prefix +Primary prefix + Word root + Primary suffix + Secondary suffix

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

No. of Carbon Atoms	Word Root
1	Meth
2	Eth
3	Prop
4	But
5	Pent
6	Hex
7	Hept
8	Oct
9	Non
10	Dec

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

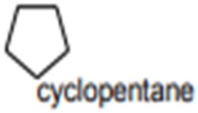
Bond Type	Suffix
All single bonds	–ane
One double bond	–ene
One triple bond	–yne

3.Secondary Suffix : A secondary suffix is always added to the primary suffix to indicate the nature of the functional group present in the organic compounds. Secondary suffix of some important functional groups are given below.

Functional Group	Group Formula	Suffix Used
Alcohol	–OH	–ol
Aldehyde	–CHO	–al
Ketone	–CO–	–one
Carboxylic acid	–COOH	–oic acid
Ester	–COOR	–oate
Ether	–O–	Alkoxy Alkane
Amine	$-NH_2$	–amine
Amide	$-CONH_2$	–amide

4.Primary prefix : A primary prefix is used simply to distinguish cyclic from acyclic compounds. For example, in case of carbocyclic compounds.(cyclic compounds containing only carbon atoms in the ring.), a primary prefix, cyclo is used immediately before the word root.

Thus



Cyclo + Pent + ane = cyclopentane

Primary prefix + word root + primary suffix = IUPAC

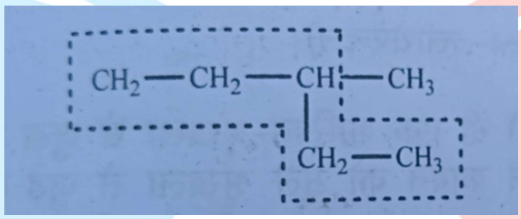
5. Secondary Prefix : In IUPAC system of nomenclature, certain groups are not considered as functional groups but instead are treated as substituents. These are called secondary prefixes and are added immediately before the word root (or the primary prefix in case of carbocyclic compounds) in alphabetical order to denote the side chains or substituent groups. The secondary prefixes for some groups which are always treated as substituents groups

Substituent / Group	Prefix
$-CH_3$	Methyl
$-C_2H_5$	Ethyl
$-C_3H_7$	Propyl
$-Cl$	Chloro
$-Br$	Bromo
$-F$	Fluoro
$-I$	Iodo
$-NO_2$	Nitro

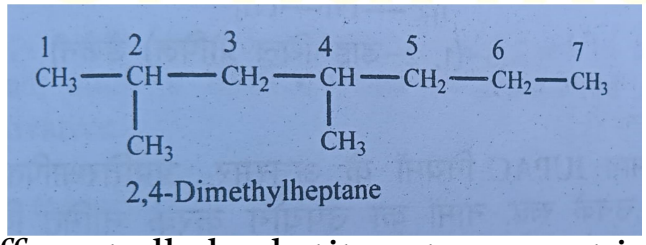
Rules Governing IUPAC Nomenclature of Branched Chain Alkanes.

Branched chain alkanes can be named by the given rules of IUPAC nomenclature system:

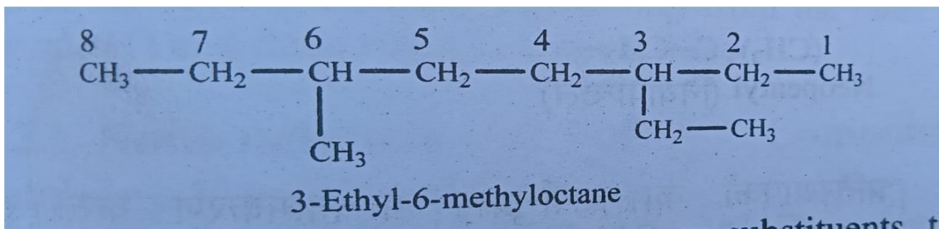
1. The longest continous chain of carbon atoms is identified as the parent chain and the compounds is considered its derivative.



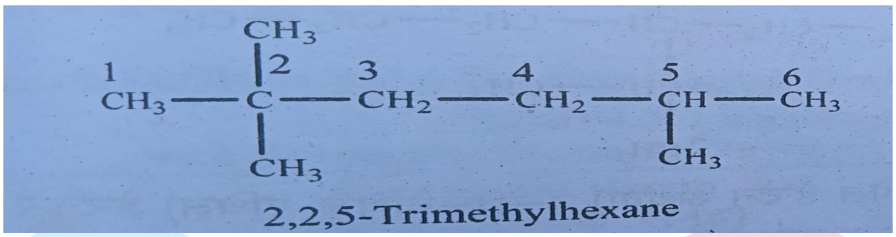
2. The carbon atom in the parent chain are numbered from one end so that the substituent carrying carbon atoms receive the lowest numbers.
3. For naming the organic compounds the position of each substituent and its name of parent alkane.



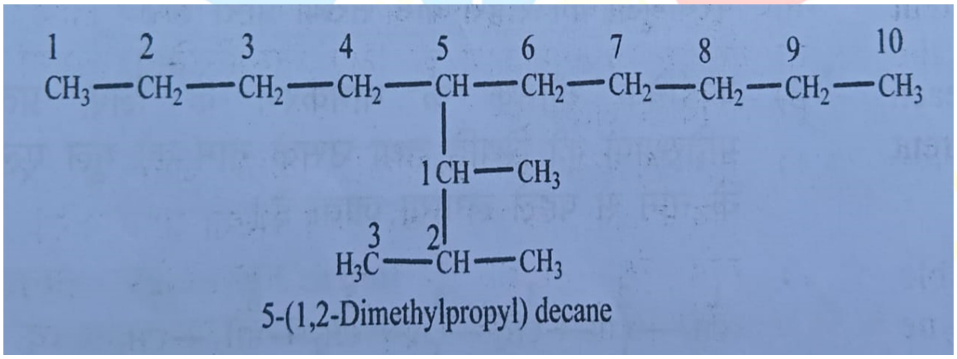
4. The names of different alkyl substituents present in the parent chain are written alphabetically
5. If the parent chain has two or more substituents at equivalent position the first substituent in the alphabetical order is given the lowest number.



6. In the presence of two or more same substituent their number position is sepersted by commas and the appropriate predix-di, tri, tetra, etc., are added to the name of each.

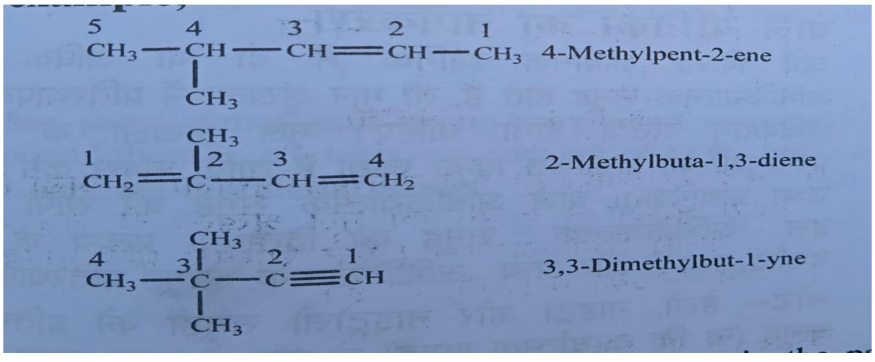


7. If the substiturnt also carries a branched chain the carbon in the chain are numbered separately beginning from the carbon attached to the parent chain. The names of such complex substituents are written within brackets.



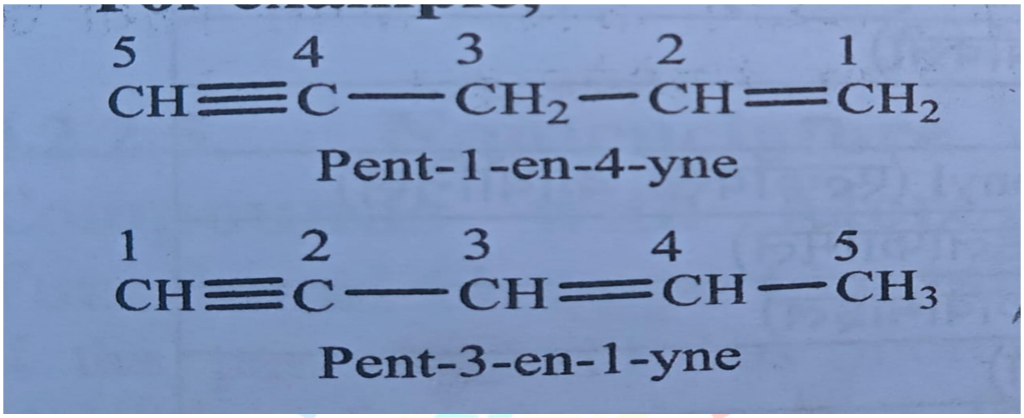
Nomenclature of Alkenes and Alkynes

Alkene and alkyne are assigned IUPAC names derived from the corresponding alkane. In the IUPAC name of alkene, the suffix -ane is replaced with ene; while in alkyne, ane is replaced with -yne.



If double as well as triple bonds are present in the parent chain, following rules are considered for naming the compound.

1) Parent chain is numbered so, that the double and triple bonds receive the lowest numbers.
2) If possible lowest number is assigned to the double bond, such a hydrocarbon is considered an alkyne derivative.



Nomenclature of compound Containing Functional Groups

→ The functional group (apart from C=C and C=C) present in a molecule is written by adding secondary suffix after the primary suffix. The 'e' terminal of the primary suffix is removed before the secondary suffix is added if its name begins with a, i, o, u, or y.

Nomenclature of Compounds with More than One Functional Group

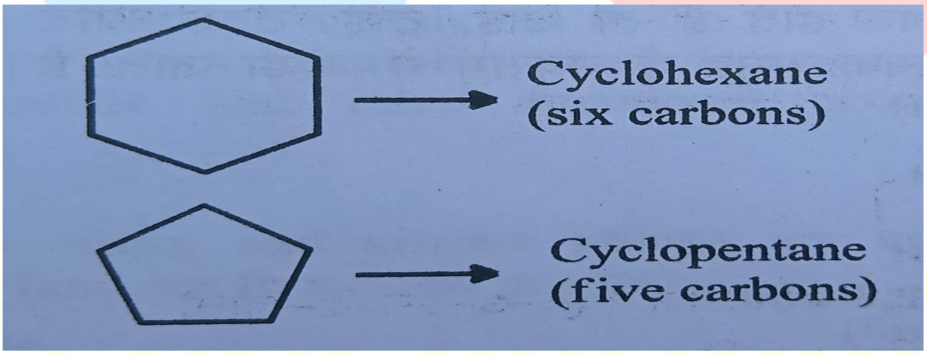
→ If an organic compound has two or more different functional groups, then the parent chain must have maximum number of Substituents. The carbon atoms of parent chain are numbered so that lowest number is assigned to the functional group of higher priority. This functional group is represented with a secondary suffix and other functional groups are the substituents.

Nomenclature of Alicyclic Compounds

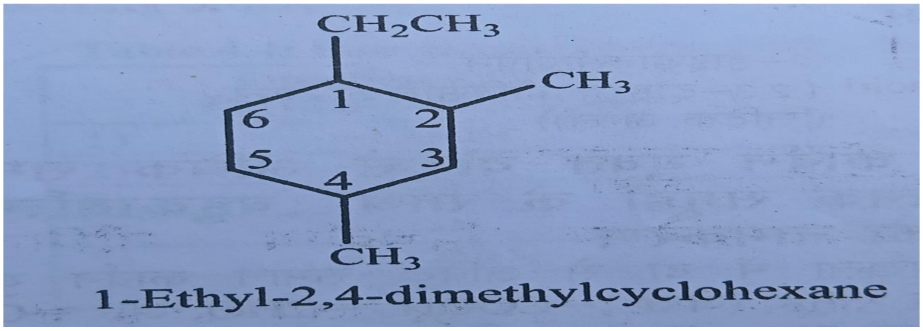
Organic Compounds having closed chain compounds and resembling with aliphatic compounds in their properties are referred as alicylic compounds Cycloalkanes , Cycloalkenes and non aromatic carbocyclic compounds are classified as alicyclic compounds

Alicylic compounds can be named based on the following rules :

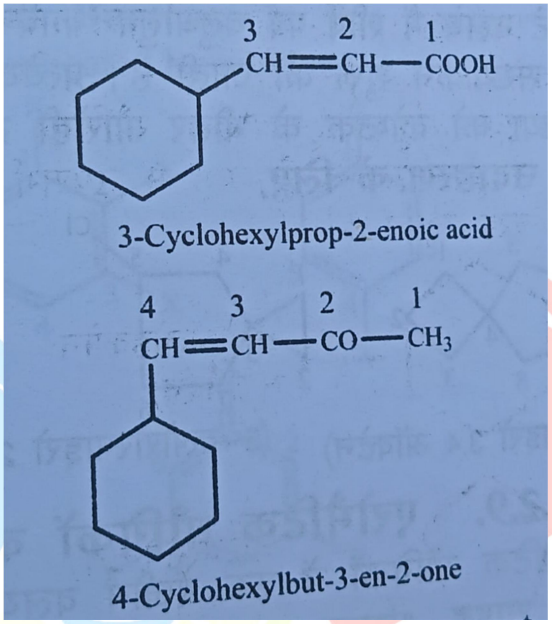
1) A saturated monocyclic compound is named prefix cyclo- to the name of the corresponding cycloalkane.



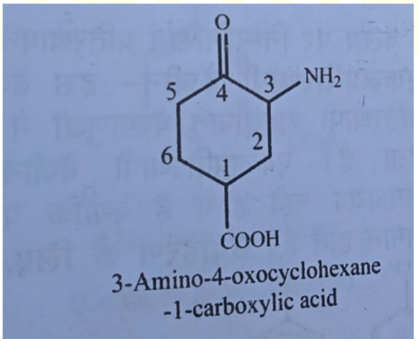
2) In the presence of two or more substituents, beginning from the one coming first in alphabetical order numbering is continued up to the last substituent so that it receives the lowest number.



3) In case, a functional group is attached to the side chain, the compound is considered as acyclic (irrespective of the ring size); while the alicyclic ring is a substituent.

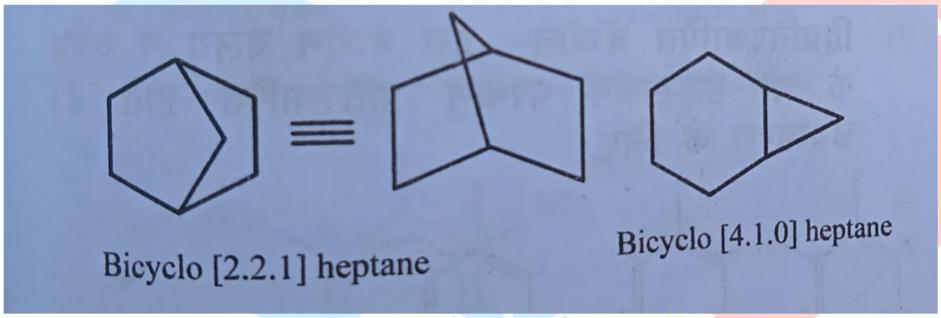


4) In case, the functional groups form a part of the ring system, the functional groups of highest priority are assigned with lowest number.



Nomenclature of Bicyclic Compounds

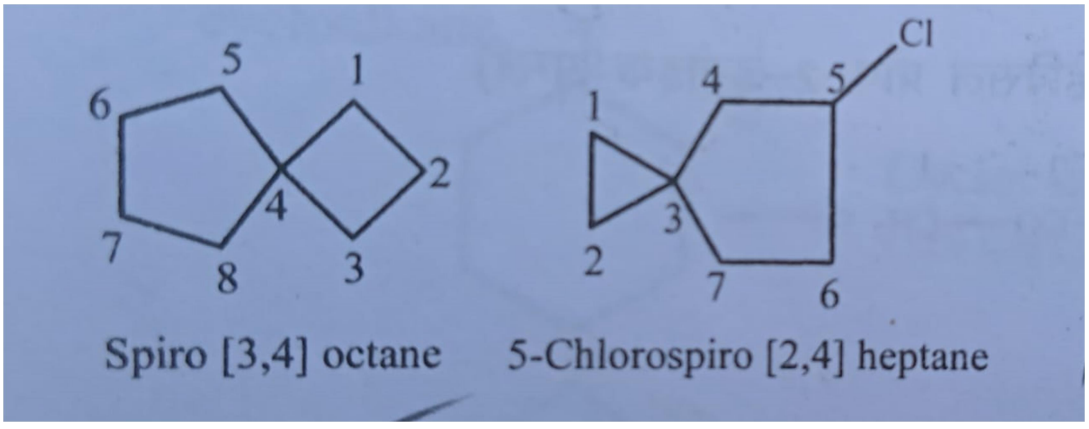
→ Bicyclic compounds have two fused rings joined by two tertiary carbon atoms. While naming these compounds, the alkane name (containing the same number of carbon as the bicyclic compound) is added after the prefix bicyclo- .The number of carbons in each of the three bridges is given within the brackets in descending order. For example,



Nomenclature of Spiro Compounds

→ Spiro compounds have two rings joined by a common quatermary carbon at the apex. While naming these compounds the name of the alkane (containin same number of carbons as part of the ring term system (s) is added: after the prefix spiro-.

→ Numbering is started from the carbon next to the quaternary carbon at the apex in the smaller ring Number of carbons in each bridge is written with in the brackets in ascending order for Example

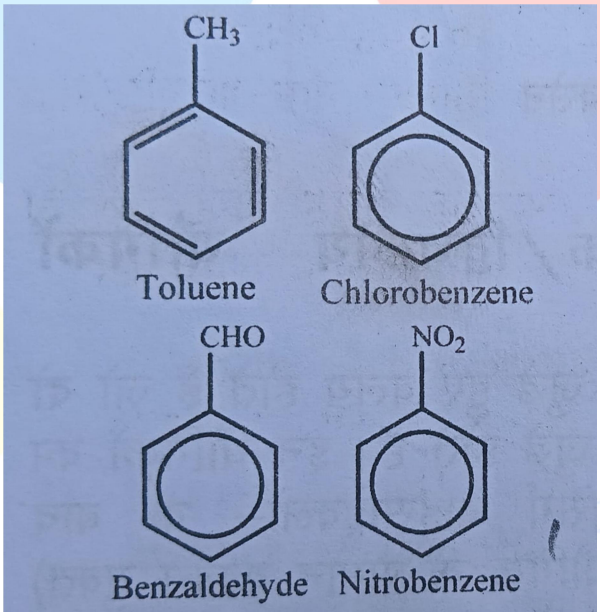


Nomenclature of Aromatic Compounds

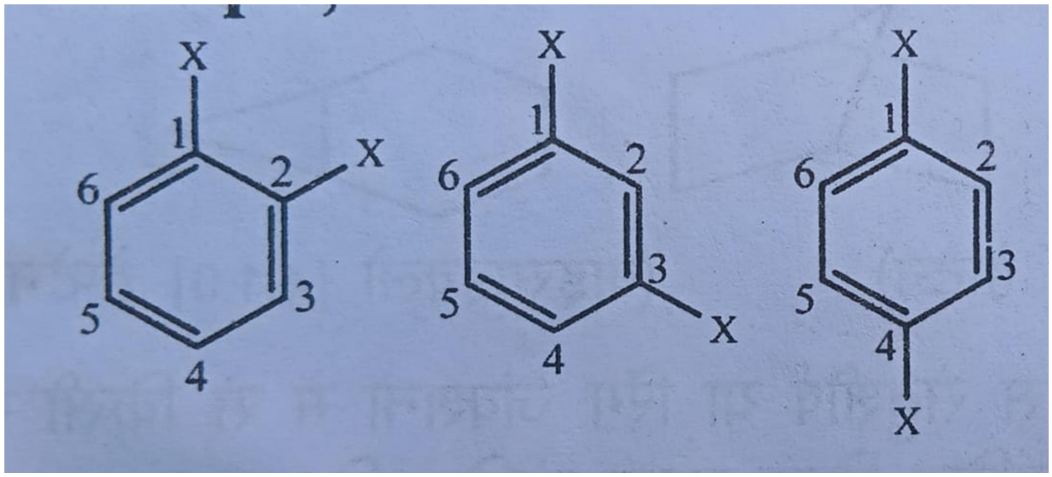
Aromatic compounds have a benzene ring and a Side chain or substituent (the group attached to benzene ring).

Follwing substitutions are possible on benzene ring

- **Monosubstituted Benzene:** In this benzene ring, a substituent replaces one of the hydrogen atoms. Monosubstituted benzene ring has no isomer as the nuclear carbons are all similar. For example.



- **Disubstituted Benzene:** In this benzene ring, two hydrogen atoms of the ring are substituted. For example,



Isomerism

→ Isomerism is the phenomenon in which more than one compounds have the same chemical formula but different chemical structures. Chemical compounds that have identical chemical formula but differ in properties and the arrangement of atoms in the molecule are called isomers.

→ Therefore, the compounds that exhibit isomerism are known as isomers.

→ The word "isomer" is derived from the Greek words "isos" and "meros", which mean "equal parts".

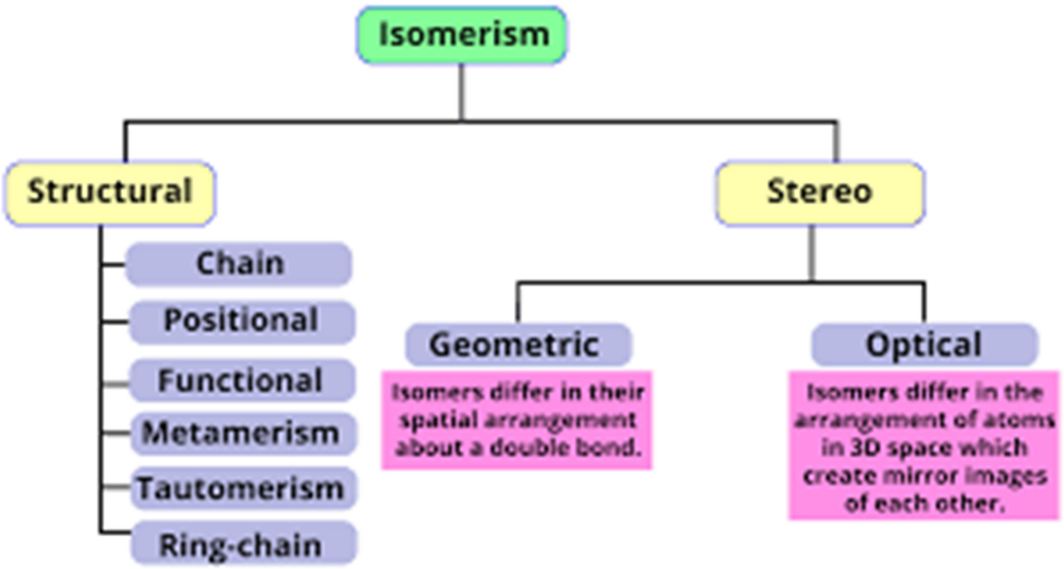
→ This term was coined by the Swedish chemist Jacob Berzelius in the year 1830.

Types of Isomerism

There are two primary types of isomerism, which can be further categorized into different subtypes. These primary types are

1. Structural Isomerism
2. Stereoisomerism.

The classification of different types of isomers is illustrated below.



Structural Isomerism

→ Structural Isomerism is commonly referred to as constitutional isomerism.

→ The functional groups and the atoms in the molecules of these isomers are linked in different ways.

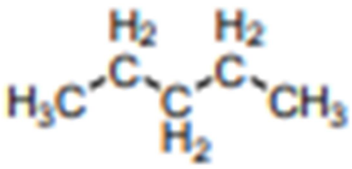
→ Different structural isomers are assigned different IUPAC names since they may or may not contain the same functional group.

→ The different types of structural isomerism are discussed below.

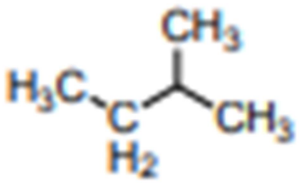
1. Chain Isomerism
2. Position Isomerism
3. Functional Isomerism
4. Metamerism
5. Tautomerism
6. Ring Chain isomerism

1. Chain Isomerism :

→ It is also known as skeletal isomerism. The components of these isomers display differently branched structures. Commonly, chain isomers differ in the branching of carbon. An example of chain isomerism can be observed in the compound C5H12, as illustrated below



Pentane



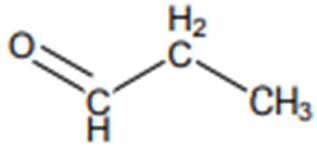
Isopentane

2. **Positional Isomerism :**

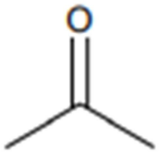
→ The positions of the functional groups or substituent atoms are different in position isomers. Typically, this isomerism involves the attachment of the functional groups to different carbon atoms in the carbon chain. An example of this type of isomerism can be observed in the compounds having the formula C_3H_7C

3. **Functional Isomerism :**

→ It is also known as functional group isomerism. As the name suggests, it refers to the compounds that have the same chemical formula but different functional groups attached to them. An example of functional isomerism can be observed in the compound C_3H_6O



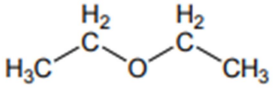
Propanal



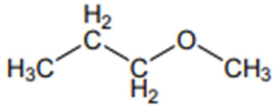
Propanone

4. **Metamerism :**

→ This type of isomerism arises due to the presence of different alkyl chains on each side of the functional group. It is a rare type of isomerism and is generally limited to molecules that contain a divalent atom (such as sulfur or oxygen), surrounded by alkyl groups. Example: $C_4H_{10}O$ can be represented as :



ethoxyethane



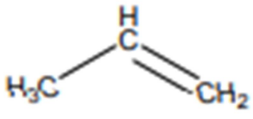
methoxy-propane

5. Tautomerism :

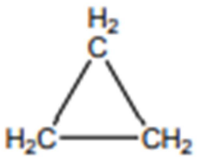
→ Tautomerism is a dynamic equilibrium between two compounds with same molecular formula. A tautomer of a compound refers to the isomer of the compound which only differs in the position of protons and electrons. Typically, the tautomers of a compound exist together in equilibrium and easily interchange. It occurs via an intramolecular proton transfer. The most common form of tautomerism is keto-enol tautomerism. A carbonyl compound containing at least one α-hydrogen atom is converted to an enol by the transfer of an α-hydrogen onto the oxygen atom. For example Keto and enol form of Acetone.

6. Ring Chain Isomerism :

→ Compounds having the same molecular formula but possessing open chain and cyclic structures are called ring chain isomers and the phenomenon is called ring-chain isomerism. For example propene and cyclopropane are ring chain isomers.



Propene



Cyclopropane