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# Unit - 1

## Classification, Nomenclature and Isomerism

- Organic chemistry is the branch of chemistry which deals with carbon containing compounds.
- Carbon atoms show highest catenation property. Carbon atoms form chains and rings of various sizes and branching.
- The various compounds of different sizes and structures corresponds to different physical and chemical properties.
- Organic chemistry holds much importance in technological world. The various dyes, pharmaceuticals, paper, paints, pesticides, insecticides, petroleum-based products, rubber tyres etc. all come under organic chemistry.
- Organic chemistry is a hugely important field in technology: it's the chemistry of dyes and pharmaceuticals, paper and ink, paints and plastics, gasoline; it's the chemistry of the food we eat and the clothes we wear.
- Organic chemistry is critical in biology and medicine. Apart from water, biological creatures are mostly composed of organic compounds; the molecules of "molecular biology" are organic compounds.
- Organic chemistry also includes carbon compounds such as cholesterol and polyunsaturated fats, growth hormones and steroids, insecticides, and many others. In addition to carbon and hydrogen, organic molecules include a vast variety of medicinal compounds that contain other heteroatoms such as O, N, S, and so on in their chemical structures.
- These compounds have wide-ranging therapeutic effect such as anti-malarial, anti-inflammatory, anti-cancer, anti-viral, anti-fungal, and so on.

### Nomenclature of Organic Compounds

Two general ways of naming organic compounds have been in practice:

#### 1. Trivial System

In which the compounds are named after the source from which they are obtained or from their characteristic property.

For example:

HCOOH -Formic acid (red ants)

CH<sub>3</sub>COOH-Acetic acid (acetum-vinegar)

**2. IUPAC system: (International Union of Pure and Applied Chemistry)**

It is most scientific and universally accepted used for nomenclature of organic compounds. Certain set of rules are to be followed for assigning IUPAC names of various organic compounds. The names assigned by following IUPAC rules are termed as systematic names. The name of the compound obtained by adding suffix and prefix to the name of the unbranched hydrocarbons. The base of the name indicates the length of the chain or ring i.e., the number of carbon atoms present in the parent compound. The suffix is added to parent name which indicates the type of functional group present in the parent chain. Prefix is used to indicate the substituent present in the organic compound.

The IUPAC name of the compound consists of:

- Prefix
- Word root
- Primary suffix
- Secondary suffix

substituent group	Prefix
-F	Fluoro
-Cl	Chloro
-Br	Bromo
-I	Iodo
-NO <sub>2</sub>	Nitro
-CH <sub>3</sub>	Methyl
-C <sub>2</sub> H <sub>5</sub>	Ethyl
-C <sub>3</sub> H <sub>7</sub>	Propyl

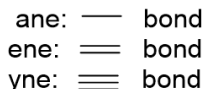
**Word Root**

Number of Carbons	Name
1	meth
2	eth
3	prop
4	but
5	pent
6	hex
7	hept
8	oct
9	non
10	dec
11	undec
12	dodec

It indicates the number of carbon atoms in the longest possible chain.

**Primary Suffix:**

Primary suffix indicates the type of carbon-carbon bond in the organic compound.



**Secondary suffix:** It represents the functional group if present in an organic molecule and is attached to the primary suffix while writing the IUPAC name. Priorities of Substituents and Functional Groups LISTED HERE FROM HIGHEST TO LOWEST PRIORITY. Many organic compounds contain more than one functional group. In those cases the functional group of highest priority is termed as suffix and is known as principal group. The functional group of lowest priority is known as junior group and is added as prefix. The following order of priority is used for selecting the principal and functional group:

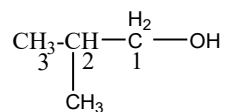
Carboxylic acids > sulphonic acids > acid anhydrides > esters > acid halides > amides > nitriles > aldehydes > ketones > alcohols > amines > ethers

Functional group	Prefix name	Suffix name
Carboxylic acid	carboxy	-oic acid
Ester	Alkoxy carbonyl	-oate
Amide	Amido	-amide
Nitrile	Nitrile	cyano
Aldehyde	Formyl	-al
Ketone	Oxo	-one
Alcohol	Hydroxy	-ol
Amine	Amino	-amine
Ether	Alkoxy	-
Alkyl Halide	Halo	-

IUPAC = prefix + word root + primary suffix + secondary suffix

Writing IUPAC name of an aliphatic compound

Eg:



**Word root:** prop

**Prefix:** methyl

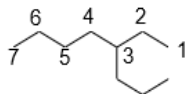
**Primary suffix:** ane

**Secondary suffix:** ol

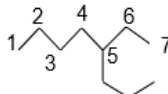
**IUPAC name-** 2-Methyl-1-propanol

## Rules of Writing Iupac Names

1. Select the largest chain



Side chain is at C<sub>3</sub>  
(right)

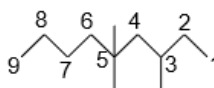


Side chain is at C<sub>5</sub>  
(left)

2. Numbering of carbon is done from the side in order to give least possible number to the side chain. Side chain derived from alkane is called alkyl. Alkyl group can be primary, secondary and tertiary.
- The prefix n-(normal) refers to a straight chain alkyl, without any branching or cross links in the chain.
  - The prefix iso is used when all carbon atoms except one are present in straight continuous chain.
  - The prefix s- is read as secondary, indicates linking at a secondary carbon that is, one bound to two carbons.
  - The prefix t- is read as tertiary to indicate attachment at a tertiary carbon-that is one bound to three other carbons.
3. If more than one side is present, sum of the positions should be minimum while numbering the carbon chain



sum of positions:  $5+5+7=17$   
(wrong)

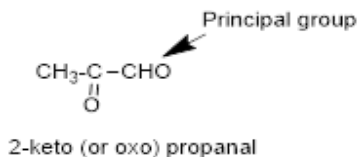


sum of positions:  $3+5+5=13$   
(right)

- If two different alkyl groups are at equal positions from each other end, numbering is done from the side of the smaller alkyl group.
- When the substituents are other than alkyl groups, numbers are assigned in the alphabetical order.
- When a compound contains a functional group, the lowest number is assigned to the functional group and to the substituent, even if it violates the minimum sum rule.
- For compounds with more than one functional group. Following order is followed in assigning principal and junior functional group:

Carboxylic acids>sulphonic acids>acid anhydrides>esters>acid  
halides>amides>nitriles>aldehydes>ketones>alcohols>amines>ethers

In the compound given below keto group is junior (prefix) functional group whereas aldehyde is principal functional group.



## Isomers

The compounds having same molecular formula but different properties due to different arrangement of atoms in the molecule are termed as isomers. There are two types of isomerism:

- **Structural Isomerism**
- **Stereo Isomerism**

**Structural Isomerism:** The structural isomers are those with different atomic arrangement of molecules without regard for spatial arrangement in 3-D space. Constitutional isomerism and structural isomerism are two terms for the same thing.

In other words, while they have same molecular formula they possess different structures. This type of isomerism which arises from difference in the structure of molecules, includes:

1. **Chain or Nuclear Isomerism;**
2. **Positional Isomerism**
3. **Functional Isomerism**
4. **Metamerism**
5. **Tautomerism**

Stereochemistry is the discipline of chemistry that studies "the various spatial configurations of atoms in molecules."

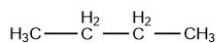
Stereochemistry is the methodical exposition of a specific topic of science and technology that generally necessitates a little detour into history. Stereochemistry is known as the "chemistry of space," since it deals with the spatial arrangements of atoms and groups in a molecule. Stereochemistry is known as the "chemistry of space," since it deals with the spatial arrangements of atoms and groups in a molecule.

**Stereochemistry may be traced back to 1842, when the French chemist Louis Pasteur discovered that tartaric acid salts obtained from a wine production vessel had the capacity to rotate plane-polarized light, but the identical salts from various sources do not. Optical isomerism gives explanation of this phenomena.**

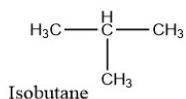
### 1. Chain Isomerism

- Isomers are chain isomers, which occur when two or more compounds have the same chemical formula but vary in the carbon atom branching. It is sometimes referred to as skeletal isomerism. These isomers' constituents have a variety of branching structures.

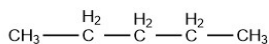
- Typically, chain isomers differ in the degree of carbon branching.



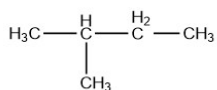
n-butane



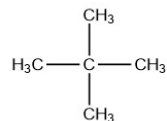
Isobutane



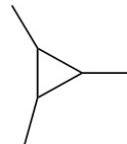
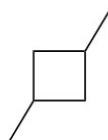
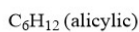
n-pentane



iso-pentane

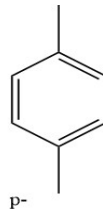
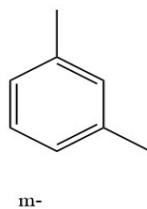
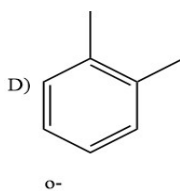
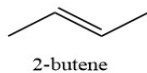
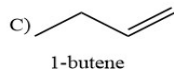
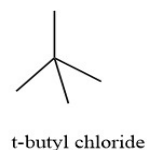
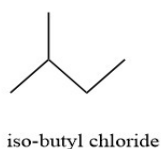
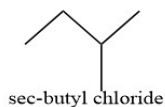
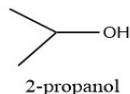
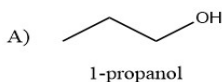


neo-pentane



## 2. Position Isomerism

Position isomers are compounds having different location of the functional group or substituent atoms. In position isomers, the locations of the functional groups or substituent atoms vary along the chain.

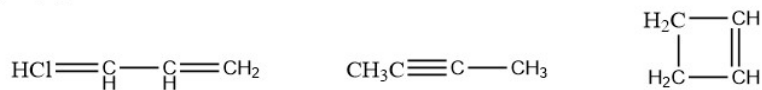


dichlorobenzene

### 3. Functional Isomerism

Isomers are functional isomers when two or more compounds have the same chemical formula but have different functional groups present in them. It is sometimes referred to as functional group isomerism.

A)  $C_4H_6$



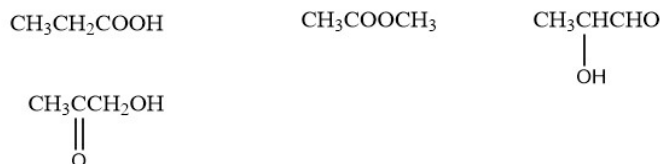
B)  $C_3H_8O$



C)  $C_3H_6O$

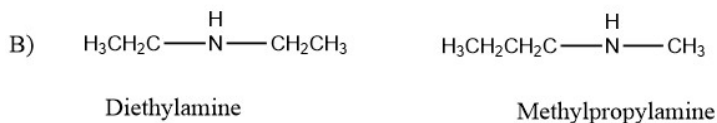
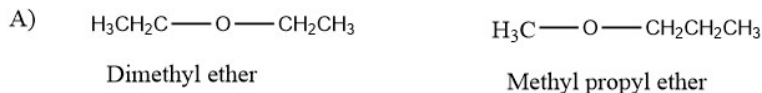


D)  $C_3H_6O_2$



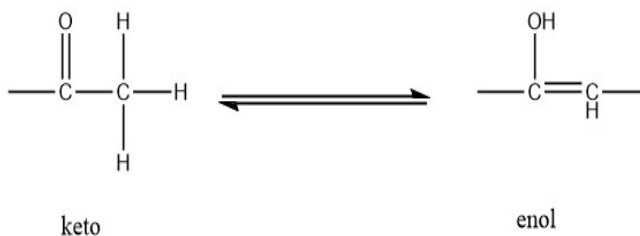
### 4. Metamerism

Metamerism arises when distinct alkyl chains are present on the either side of the functional group. It is a type of isomerism that occurs only in compounds having a divalent element (sulphur or oxygen) having alkyl groups on both the sides.

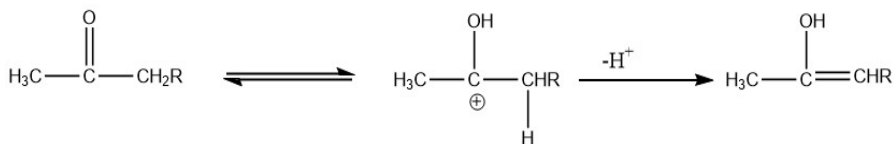


## 5. Tautomerism

Tautomers of the compound have different location of protons and electrons. Carbonyls exhibit keto-enol tautomerism due to the acidity of hydrogens. Tautomers are constitutional isomers that are rapidly interconverted. Under typical conditions, the equilibrium between tautomers is not only quick, but it frequently favours one of the isomers (acetone, for example, is 99.9% keto tautomer).



- The tautomers of a chemical exist in equilibrium with each other and easily exchange.
- This occurs through intramolecular transfer of proton. Keto-enol tautomerism is a prominent example. Tautomerism basically happens in the presence of a catalyst.
- Acid-catalyst: Protonation occurs first, followed by cation delocalization. The cation deprotonates at the neighbouring site.
- Deprotonation is the initial step in the production of base catalysts. Instead of cation delocalization, anion delocalization occurs, followed by protonation to a new anion location.

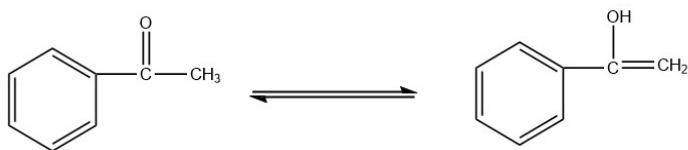
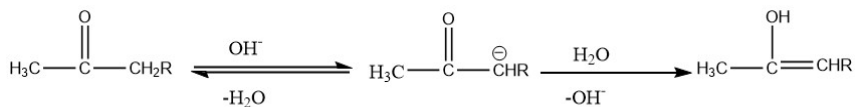


### ACID CATALYSED CONVERSION

One of the most important characteristics of tautomerism is that it increases the stability of the chemical compound. In this process, a hydrogen atom is exchanged between two other atoms while creating a covalent bond to either one. Structural requirement of Tautomerism are as follows:

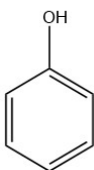
- ✓ Compounds comprise polar molecules and functional groups with weakly acidic groups.
- ✓ It has no influence on bond length or other characteristics.
- ✓ It often occurs in planar or non-planar molecules.





keto

enolic form



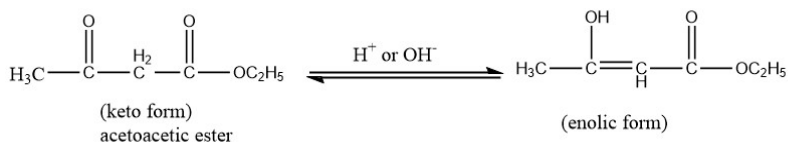
enolic form

keto form



Cyanic acid

Isocyanic acid

(keto form)  
acetoacetic ester

(enolic form)

### Tautomerism Types

Emil Erlenmeyer, a scientist, developed the rule for tautomerism in the 1880s. He was among the first to explore the keto-enol tautomerism. According to this rule, the hydroxyl group in all alcohols generates ketones or aldehydes when it is directly connected to a double-bonded carbon atom. This was attributable to the increased stability of the keto form.

There are other forms of tautomerism, but keto-enol tautomerism is the most common. One structure in this form is a ketone, while the other is an enol. By using acid or basic catalysts, both tautomeric forms can be interconverted to one other. Enolization is the process of converting a ketone to an enol.

**Prototropy**

It is a form of tautomerism caused by the compound's acid-base behaviour. The sole difference between these two versions is the location of a proton. This structure will use the same empirical formula and numbers of charges as the previous one.

**Annular Tautomerism**

An annular tautomerism occurs when a proton occupies two or more positions in a heterocyclic system. If an open structure in tautomerism is converted to a ring structure owing to proton delocalization, then such tautomers are known as ring-chain tautomers. Ring-chain tautomerism is also studied in glucose.

**Valence Tautomerism**

Valence tautomerism is a kind of tautomerism in which single and double bonds are continuously formed and broken in the compound without any movement of groups or atoms. It differs from the preceding form of tautomerism in that it occurs quickly.

There is a shift in geometrical structure but no change in canonical resonance structure or mesomers in this tautomerism.

**MCQs**

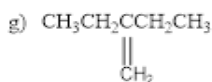
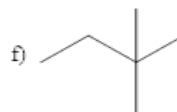
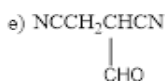
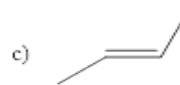
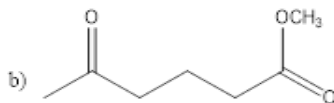
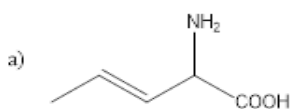
1. Give the IUPAC name of given compound



- |                      |                      |
|----------------------|----------------------|
| (a) Pent-1-en-4-yne  | (b) Pent-4-en-1-yne  |
| (c) Pent-5-yne-1-ene | (d) Pent-1-yne-5-ene |
2. The number of sigma and pi bond in the compound pent-3-en-1-yne
- |           |           |
|-----------|-----------|
| (a) 10, 3 | (b) 3, 10 |
| (c) 9, 4  | (d) 8, 3  |
3. An isomer of ethanol
- |                    |                   |
|--------------------|-------------------|
| (a) Methanol       | (b) Diethyl ether |
| (c) Dimethyl ether | (d) Acetone       |
4. Compounds having same molecular formula but different structures are called:
- |                        |                      |
|------------------------|----------------------|
| (a) Structural isomers | (b) Molecular isomer |
| (c) Optical isomers    | (d) Position isomers |
5. A monocarboxylic is functional isomer of
- |           |             |
|-----------|-------------|
| (a) Ether | (b) Amine   |
| (c) Ester | (d) Alcohol |

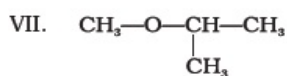
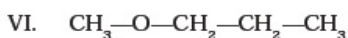
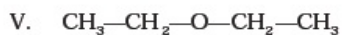
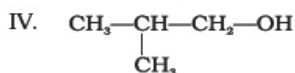
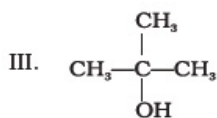
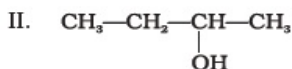
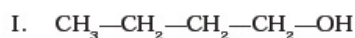


4. Write IUPAC names of following organic compounds.



### Long Answer Questions

1. In the structures given below identify the following:



- Which of the above compounds form pairs of metamers?
- Identify the pairs of compounds which are functional group isomers.
- Identify the pairs of compounds that represents position isomerism.
- Identify the pairs of compounds that represents chain isomerism.
- What do you mean by structural isomers? Discuss the various type of structural isomers with its examples.