Name of Unit	Classification, Nomenclature and Isomerism
Subject /Course Name	Pharmaceutical Organic Chemistry-I
Subject/Course ID	BP202T
Class: B.Pharm.Semester	II
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Learning Outcome of Module 02

LO	Particular	Course Outcome Code
LO1	To gain knowledge about organic compounds and its classification.	BP202.3
LO2	To understand different nomenclature system.	BP202.1
LO3	To gain knowledge of different rules for the nomenclature of organic compounds with example.	BP202.1
LO4	To get the knowledge about Isomerism and its classification.	BP202.3

Content Table

Topic
• Introduction of Organic Chemistry and Organic Compounds • Importance of Organic Chemistry • Classification of organic compounds • Nomenclature of Organic Compounds • Common System of Nomenclature of Organic Compounds • IUPAC System of Nomenclature of Organic Compounds • Isomerism and its types • Structural isomerism in organic compounds.

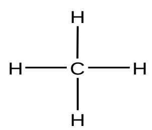
INTRODUCTION OF ORGANIC CHEMISTRY

Organic chemistry *is a branch of chemistry that studies the* ***structure, properties and reactions of organic compounds****, which contain carbon in covalent bonding.*

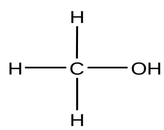
Introduction of Organic Compounds

Earlier people thought that compounds which are obtained from plants and animals are organic compounds and compounds which are obtained from minerals, non-living sources are termed as inorganic compounds. However, the modern definition of organic compounds is a bit different to this.

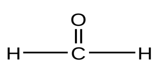
Organic compounds are generally any chemical compounds that contain carbon-hydrogen bonds. Due to carbon's ability to catenate (form chains with other carbon atoms), millions of organic compounds are known. The study of the properties, reactions, and syntheses of organic compounds comprise the discipline known as organic chemistry. For historical reasons, a few classes of carbon-containing compounds (e.g., carbonate salts and cyanide salts), along with a few other exceptions (e.g., carbon dioxide), are not classified as organic compounds and are considered inorganic. Some Examples of Organic Compounds are Given Below:-



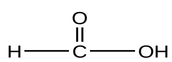
Methane



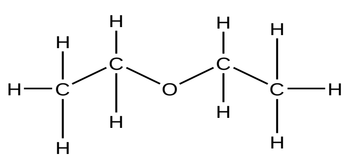
Methyl alcohol



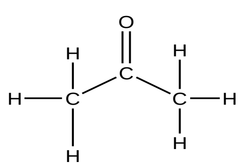
formaldehyde



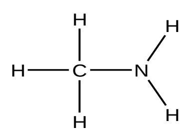
formic acid



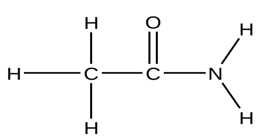
Diethylether



Acetone

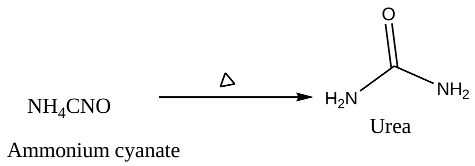


methylamine



Acetamide

The first organic compound prepared in the laboratory is **urea**. ***German chemist Friedrich Wohler prepared urea in a laboratory in 1828 from ammonium cyanate***.



Importance of organic chemistry

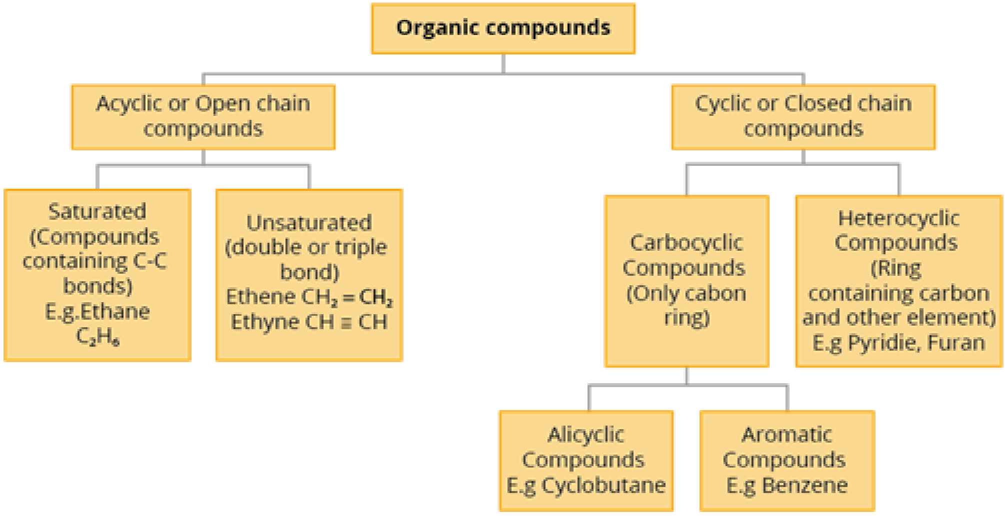
Organic chemistry is important because it is the study of life and all of the chemical reactions related to life. Several careers apply an understanding of organic chemistry, such as doctors, veterinarians, dentists, pharmacologists, chemical engineers, and chemists. No field of science is so closely related with our daily activities as is organic chemistry. The food we eat mainly organic in nature. The changes which this food undergoes in our bodies, are organic chemical reactions. Metabolism, growth and Maintanance of our bodily functions involves organic chemistry.

- Building units of all living matter: Carbohydrates, proteins, fats.
- All foods are organic compounds.
- Photosynthesis is a reaction that makes carbon a part of our food. Carbon is passed along through food and sugar from photosynthesis is modified and combined with other materials.
- Dead organisms are food for other organisms or are buried in the earth and converted to fossil fuels like peat, coal and petroleum.
- Petroleum is the source of fuel and starting material for plastics, fabrics and industrial chemicals.

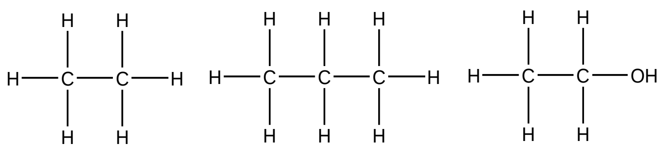
Classification of Organic Compounds

Organic compounds are classified into three main groups depending on the nature of carbon chains.

- **Acyclic compounds or Aliphatic compounds**
- **Carbocyclic compounds**
- **Heterocyclic compounds**

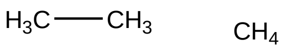


Aliphatic compounds (open chain compounds): Compounds which consist of open-chain of carbon atoms are called aliphatic compounds. There is no limit to the number of atoms involved. Examples are



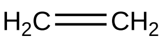
ethane propane ethanol

(a) Saturated Aliphatic Compounds: A compound is said to be saturated if it contains only C-C single bonds. Example are



Ethane Methane

(b) Unsaturated aliphatic compounds: A compound is said to be unsaturated if it contains C=C or multiple bonds. Examples are,



ethene

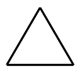
2. Closed or Cyclic Compounds: Compounds which consist of closed-chain of carbon atoms are called closed or cyclic compounds. These are two types.

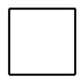
(a) Carbocyclic Compounds

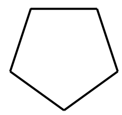
(b) Heterocyclic compounds

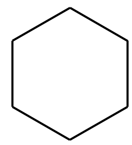
(a) Carbocyclic compounds: Cyclic compounds which consist only of carbon atoms are called cyclic or carbocyclic compounds. These are further two types.

1.**Alicyclic compounds**: Compounds which consist only of carbon atoms are called cyclic or alicyclic compounds. Examples are

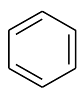

Cyclopropane

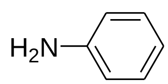

Cyclobutane


Cyclopentane

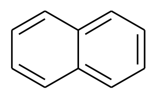

Cyclohexane

2. Aromatic Compounds: Benzene and all compounds that have structures and chemical properties resembling benzene are called aromatic compounds. Example are:

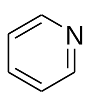

benzene



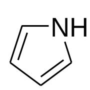
aniline


naphthalene

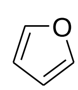
(b) Heterocyclic compounds: Cyclic compounds in which the ring atoms are of carbon and some other elements (example N,O and S) are called heterocyclic compounds. Examples are



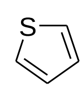
pyridine



pyrrole



furan



thiophene

NOMENCLATURE OF ORGANIC COMPOUNDS There are **two system** of naming of organic compounds.

Nomenclature of Compounds

Common or Trivial system **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 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 nomenclature of organic compounds refers to the systematic approach taken for the nomenclature of organic compounds as per the recommendation of the International Union of Pure and Applied Chemistry (often abbreviated to IUPAC).

According to the **Guidelines set by IUPAC**, the nomenclature of compounds must follow these steps:

The Longest Chain Rule: The parent hydrocarbon must be identified and subsequently named. The parent chain belonging to the compound in question is generally the longest chain of carbon atoms, be it in the form of a straight chain or a chain of any other shape.

The Lowest Set of Locants: The carbon atoms belonging to the parent hydrocarbon chain must be numbered using natural numbers and beginning from the end in which the lowest number is assigned to the carbon atom which carries the substituents.

Multiple instances of the same substituent: Prefixes which indicate the total number of the same substituent in the given organic compounds are given, such as di, tri, etc.

Naming of different substituents: In the organic compounds containing multiple substituents, the corresponding substituents are arranged in alphabetical order of names in the IUPAC nomenclature of organic compounds in question.

The naming of different substituents present at the same positions: In the scenario wherein two differing substituent groups are present at the same position of the organic compound, the substituents are named in ascending alphabetical order.

Naming Complex Substituents: Complex substituents of organic compounds having branched structures must be named as substituted alkyl groups whereas the carbon which is attached to the substituent group is numbered as one. These branched and complex substituents must be written in brackets in the IUPAC nomenclature of the corresponding compounds.

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

- **Word root**
- **Primary Suffix**
- **Secondary Suffix**
- **Primary Prefix**
- **Secondary Prefix** Thus, a complete IUPAC name of an organic compound consists of the following parts :

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.

Root word : According to number of carbon's in parent C–chain.

No. of C atom	Word root
C_1	Meth
C_2	Eth
C_3	Prop
C_4	But
C_5	Pent
C_6	Hex
C_7	Hept
C_8	Oct
C_9	Non
C_{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 :

S.No	Type of Carbon chain	Primary Suffix	General Name
1.	Saturated	ane	Alkane
2.	Unsaturated with double bonds	ene	Alkene
3.	Unsaturated with triple bond	yne	Alkyne

If the parent carbon chain contain two, three or more double or triple bond, numerical prefix such as di (for two), tri (for three), tetra (for four) etc. are added to the primary suffix. For example.

S.No	Type of Carbon chain	Primary Suffix	General Name
1.	Unsaturated with two double bonds	diene	Alkadiene
2.	Unsaturated with two triple bond	diyne	Alkdiyne

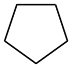
3.Secondary Suffix : A secondary suffix is always added to the primary suffix to indicate the nature of the functional group present in the organic compounds. Secondary suffix of some important functional groups are given below.

S. No.	Class of organic compounds	Functional group	Secondary Suffix
1	Alcohols	– OH	- ol
2	Aldehydes	–CHO	- al
3	Ketones	> C = O	- one
4	Carboxylic acids	– COOH	- oic acid
5	Acid amides	$-CONH_2$	- amide
6	Acid chlorides	– COX	- oyl halide
7	Esters	– COOR	alkanoate
8	Nitriles	– CN	- nitrile
9	Thioalcohols	– SH	- thiol
10	Amines	$-NH_2$	- amine

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

S. No.	Organic Compounds	Word root	Primary suffix	Secondary suffix	IUPAC name
1	CH_3CH_2OH	Eth	an (e)	ol	Ethanol
2	$CH_3CH_2CH_2NH_2$	Prop	an (e)	Amine	Propanamine
3	$CH_3CH_2CH_2COOH$	But	an (e)	Oic acid	Butanoic acid
4	CH_3CH_2CN	Prop	an(e)	Nitrile	Propanenitrile
5	$CH_2 = CHCHO$	Prop	en(e)	al	Propenal
6	$HC \equiv CCOOH$	Prop	yn(e)	oic acid	Propynoic acid

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.


cyclopentane

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 (regardless of the fact whether the organic compound is monofunctional or polyfunctional) are given below :

S. No.	Organic Compounds	Secondary prefix	Word root	Word root	IUPAC name
1	CH_3CH_2–Br	Bromo	eth	ane	Bromoethane
2	CH_3–NO_2	Nitro	meth	ane	Nitromethane
3	C_2H_5–OC_2H_5	Ethoxy	eth	ane	Ethoxyethane

In case of carbocylic compounds, primary prefixes are also used.

Nomenclature of Polyfunctional Compounds: In a polyfunctional compound, one of the functional groups is selected as the principal functional group while all other functional groups are treated as substituents.

Principal functional group: In a polyfunctional compound, one of the functional groups is selected as the principal functional group while all other functional groups are treated as substituents.

Functional groups according to their priorities are listed in the priority table in decreasing order i.e., Carboxylic acid with the highest priority is placed at the top while alkyne being the least in priority is placed at the bottom. The functional group which has the highest priority among all the functional groups present in an organic compound is selected as the principle functional group.

Compound Name	Formula
Carboxylic acid	-COOH
Sulphonic acid	$-SO_3H$
Ester	-COOR
Acid Chloride	-COCl
Acid Amide	$-CONH_2$
Nitrile	-CN
Aldehyde	-CHO
Ketone	-C=O
Alcohol	-OH
Phenol	$-C_6H_6OH$
Thiols	-SH
Amine	$-NH_2$
Ether	-OR
Alkene	>C=C<
Alkyne	HC=CH

All functional groups other than the principal functional group present in an organic compound are called substituents.

In the following example, **COOH** being highest in priority is selected as the principal functional group while all others are treated as substituents.

Some of the substituents with their prefixes are given below :

Secondary Functional Groups	**Prefix**
-X	Halo(Floro,Chloro,Bromo)
-OH	Hydroxy
-SH	Mercapto
-OR	Alkoxy
-NH_2	Amino
-CHO	Formyl
-C=O	Keto or Oxo
-COOH	Carboxy
-COOR	Alkoxycarbonyl or carboalkoxy
-COCl	Halocarbonyl
-CN	Cyano
-$CONH_2$	Carbomoyl or carboxamide

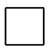
Nomenclature of Carbocyclic Compounds: Carbocyclic compounds are **two types**

1.Alicyclic Compounds

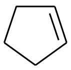
2.Aromatic Compounds

Nomenclature of Alicyclic Compounds:

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

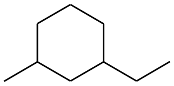


cyclobutane



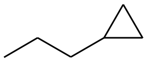
cyclopentene

(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 given the lowest possible number provided it does not violate the lowest set of locants rule. Example,



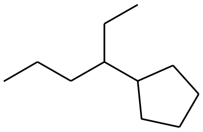
1-ethyl-3-methylcyclohexane

(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



propylcyclopropane

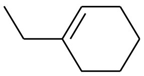
(4) The alkane chain contains greater number of carbon atoms than present in the ring, the compound is considered as the derivative of alkane and the ring is designated as substituent.



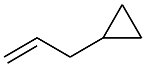
3-cyclopentylhexane

(5) (a) If ring has unsaturation and side chain is saturated then ring is selected as parent chain.

(b) If side chain has unsaturation and ring is saturated then side chain is selected as parent chain.

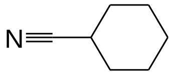


1-ethylcyclohex-1-ene



3-cyclopropyl prop-1-ene

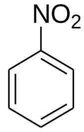
(6) When chain terminating functional group is directly attached with ring then ring is taken as parent chain & special suffix used for functional group.



cyclohexane carbonitrile

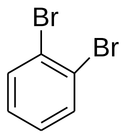
Nomenclature of Aromatic Compounds:

- According to IUPAC nomenclature of substituted aromatic compounds, the substituent name is placed as a prefix to the name of aromatic compounds.For example, a benzene ring attached to a one-nitro group.

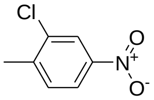


Nitrobenzene

- When more than one similar substituent group is present in the ring, they are labelled with the Greek numerical prefixes such as di, tri, tetra to denote the number of similar substituent groups attached to the ring. If two bromo- groups are attached to the adjacent carbon atoms of the benzene ring, it is named 1,2-dibromobenzene.



- When different substituted groups are attached to the aromatic compounds, the substituent of the base compound is assigned number one and then the direction of numbering is chosen such that the next substituent gets the lowest number. Substituents are named in alphabetical order. For example: when chloro and nitro groups are attached to the benzene ring, we first locate the chloro group then nitro groups.



2-chloro-1-methyl-4-nitrobenzene

- In the case of multiple substituted aromatic compounds, sometimes terms like ortho (o), meta (m) and para (p) are also used as prefixes to indicate the relative positions 1,2-; 1,3- and 1,4- respectively. For example, 1,2-Di-bromo-benzene can be named as o-di-bromo-benzene.
- When an alkane with a functional group is attached to an aromatic compound, the aromatic compound is considered as a substituent, instead of a parent. For example: when a benzene ring is attached to an alkane with a functional group, it is considered as a substituent named phenyl, denoted by Ph-.

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.**

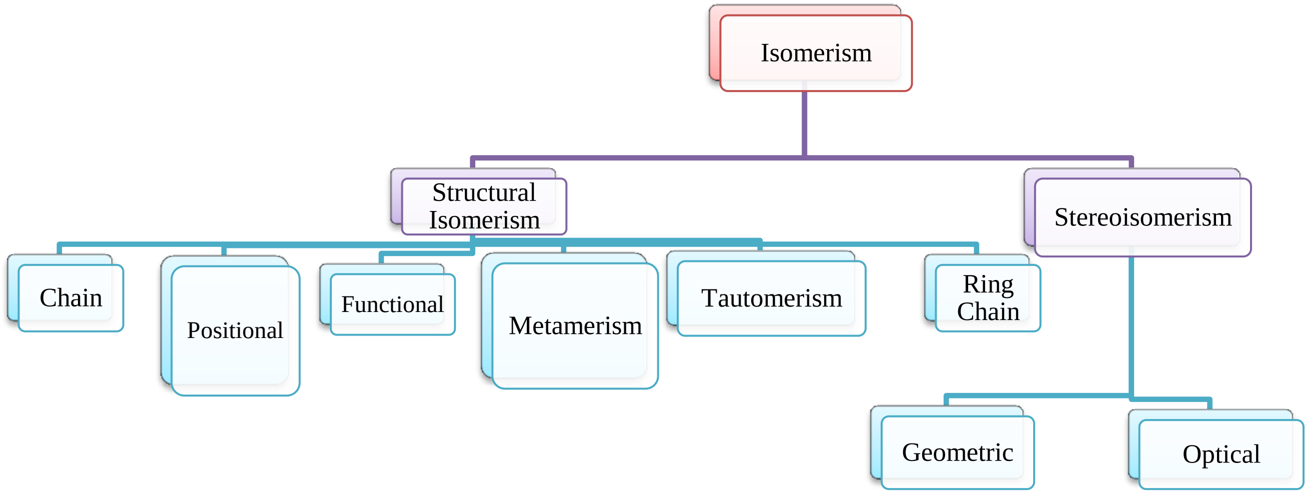
Types of Isomerism:

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.



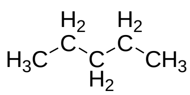
Structural Isomerism

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.

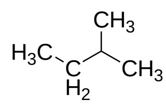
1. **Chain Isomerism**
2. **Position Isomerism**
3. **Functional Isomerism**

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 C_5H_{12}, as illustrated below



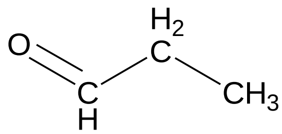
Pentane



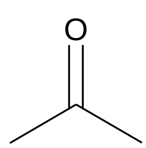
Isopentane

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.

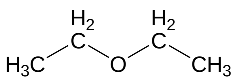


Propanal

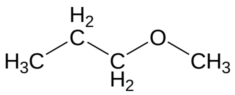


Propanone

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 :

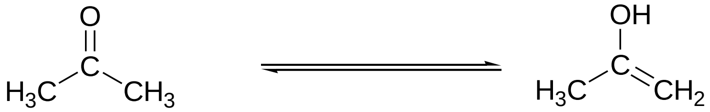


ethoxyethane

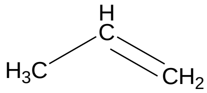


methoxy-propane

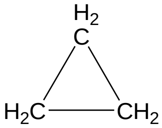
5.Tautomerism: Tautomerism is a dynamic equilibrium between two compounds with same molecular formula. A tautomer of a compound refers to the isomer of the compound which only differs in the position of protons and electrons. Typically, the tautomers of a compound exist together in equilibrium and easily 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

Very Short Answer Type Questions (2 Marks)

1. Give the structure and IUPAC name of the followings

(a)Acetone

(b)Diethyl ether

2. Give the structure and IUPAC name of the followings

(a)Isopropyl alcohol

(b)Methyl formate

3. Write the general rules of IUPAC nomenclature.

4. Define metamerism with examples?

5. Write the structure and IUPAC name of Ethyl acetoacetate.

6. Give the structure and IUPAC name of the followings

(a) Ethyl methyl ketone

(b) Diethyl ether

7. Define structural isomerism with suitable example.

8. Define functional isomerism with example.

9. Give the structure and IUPAC of 2-Bromo-3-methylhexane and Methanol.

10. What is Geometrical Isomerism?

Short Answer Type Questions (5 Marks)

1. What are Acyclic compounds? Give examples.

2. Explain classification of organic compounds.

3. What is common system of nomenclature of Organic compounds?

4. What is Isomerism?

5. Write down the structure and IUPAC names of the followings

(a) Formic acid

(b)Acetone

(c)Acetylene

(d)Ethylamine

(e)Acetaldehyde

(f)Dimethyl ether

6. Define isomerism? Classify with suitable example

Long Answer Type Questions (10 Marks)

1. What do you mean by IUPAC system of nomenclature? Give the IUPAC names of different classes of compounds.

2. Write down the structural formula of

(a) 2-Methylpentane

(b)Pentane-2-one

(c)Methyl ethyl pentane

(d)1,3-Butadiene

(e) 3-ethylbutanol

3. Explain isomerism in organic compounds.

4. Explain tautomerism and Metamerism in details with suitable.