

Chapter



4

Nomenclature of Organic Compounds



INTRODUCTION

- ✓ Organic compounds exhibit a great diversity with millions of known compounds and an infinite number of possible isomers.
- ✓ These compounds can possess distinct functional groups, different type of substituents, and variable lengths, branches and cyclic structure of carbon chains leading to a wide range of structural possibilities.
- ✓ it was a big challenge for organic chemists to establish a systematic and simplified method for naming the vast number of organic compounds in a consistent and uniform manner.
- ✓ However this challenge was successfully addressed with the introduction of IUPAC (international union of pure and applied chemistry) naming system which provides comprehensive solution for the nomenclature of organic compounds and allows chemists to identify and understand the vast array of organic compounds that exists in nature or are synthesized in the laboratory.

HYDROCARBONS AND THEIR DERIVATIVES

Organic compounds are mainly made up of carbon and hydrogen, however certain other elements such as oxygen, nitrogen, Sulphur and halogen may also be present in their structures.

Number of carbon atoms in chain	prefixes	Alkane	Alkene	Alkyne
1	Meth-	Methane		
2	Eth-	Ethane	Ethene	Ethyne
3	Prop-	Propane	Propene	Propyne
4	But-	Butane	Butene	Butyne
5	Pent-	Pentane	Pentene	Pentyne
6	Hex-	Hexane	Hexene	Hexyne
7	Hept-	Heptane	Heptene	Heptyne
8	Oct-	Octane	Octene	Octyne
9	Non-	Nonane	Nonene	Nonyne
10	Dec-	Decane	Decene	Decyne
11	Undec-	Undecane	Undecene	Undecyne
12	Dodec-	Dodecane	Dodecene	Dodecyne

HISTORY OF NOMENCLATURE

Every organic compound found on Earth possesses a distinct structural feature. Initially the names of organic compounds were assigned on the basis of origin or the person who discovered.

These specific designations are referred to as common names or trivial names.

With the rapid growth of organic chemistry, the number of compounds increased tremendously, where it became impossible to assign a common name to such an extensive range of compounds and scientists felt the need for a structural or systematic name, that one would accurately reflect the molecular structure of organic compound.

An attempt was made at Geneva conference (1892) to create unique nomenclature wherein only one official name would be assigned to each compound. In 1958, a new commission on nomenclature was appointed by the international union of pure and applied chemistry (IUPAC) for further work on the nomenclature.

This new system of nomenclature has set rules for naming organic molecules on the basis of their structures.

IUPAC SYSTEM

The systematic or scientific system for the naming of organic compound is referred as IUPAC method. This system provides distinct names for over fifteen millions reported organic compounds and can be devised for the millions of organic compounds yet to be synthesized.

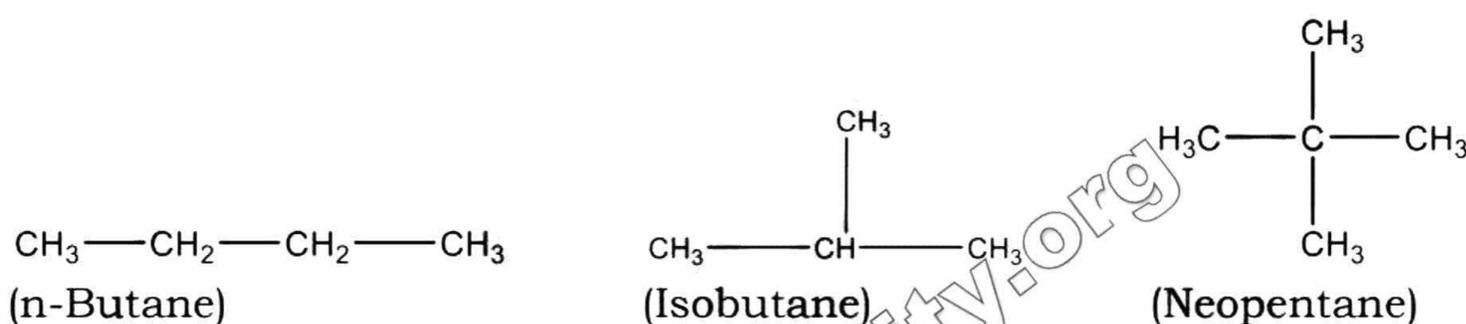
IUPAC method considers the arrangement of carbon atoms, types and positions of functional groups and other distinctive features of the compound to generate a standard name.

- 1) The general rules set for IUPAC method of naming organic compounds are as follow:
- 2) Identify the longest unbroken carbon chain within the molecule which will act as parent chain.
- 3) Allocate numerical designations to the carbon atoms within the parent chain to the terminal side, to which functional group is nearer.
- 4) Identify substituents and name them using prefix such as methyl, ethyl, methoxy, chloro, bromo etc. and mention their position in the longest carbon chain.
- 5) If any functional group is present in the molecule, name it by using appropriate suffix such as "one" for ketone, "-al" for aldehyde and "-ol" for alcohol etc.
- 6) If there are more than one functional group present in the molecule, write their name on priority basis set by priority rules i.e.
(-COOH) > (-CHO) > (C=O) > (-OH) > (-NH₂) > (-O-) > (=) > (=).

NOMENCLATURE OF ALKANES

In this system, all the carbon atoms present in the structure are included in the name, regardless of whether these carbon atoms are attached to each other in straight chain or in a branch form.

- 1) The prefix n- is utilized for alkanes where all the carbon atoms are arranged in a single uninterrupted straight chain.
- 2) The prefix Iso- is utilized if in the structure of alkane molecule one branch (e.g. CH₃) is attached to the second last carbon atom of the chain.
- 3) The prefix Neo- is utilized if two branches are attached on the second last carbon of alkanes.



IUPAC System

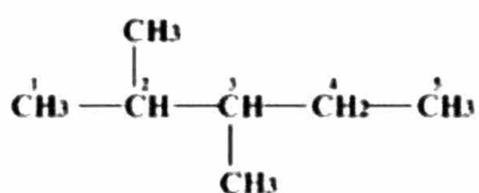
- ✓ The IUPAC names of alkane family is ended with the suffix "ane".
- ✓ The first four members of this group of organic compounds are written by their trivial names (methane, ethane, propane and butane).
- ✓ From the fifth onwards alkanes are named by prefixing the Greek numerals pent (five), hex (six), hept (seven), oct (eight) etc. indicating the number of carbons presents in the molecule to the suffix "ane",

When naming a specific alkane, by IUPAC system it is important to consider the following fundamental rules.

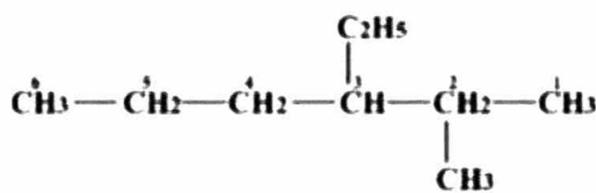
- 1) Select the longest continuous carbon chain in the molecule and number the carbon chain from one of its terminal. The name of the chain is retained as propane, butane, pentane, hexane etc.
- 2) The numbering of carbon chain should be assigned, starting from the terminal where functional group or an alkyl group (substituent) is nearest. 
- 3) If the identical substituents are attached at the same position from both ends of main carbon chain, numbering can be done from either terminal. However, if the identical substituents are attached at different positions, the numbering should be done from the side where the substituent is nearer.
- 4) When two different substituents are attached at the same position from either side of the carbon chain, the numbering of chain is determined

from the terminal where the substituent with the lower alphabetical order is nearer.

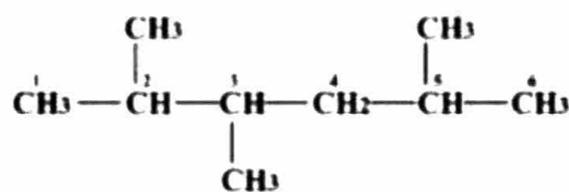
- 5) When two or more same substituents are attached to the carbon chain, indicate the quantity of each substituent by using di, tri and so forth.
- 6) Prefix cyclo is used to name cycloalkanes.



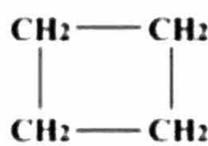
(2, 3-Dimethylpentane)



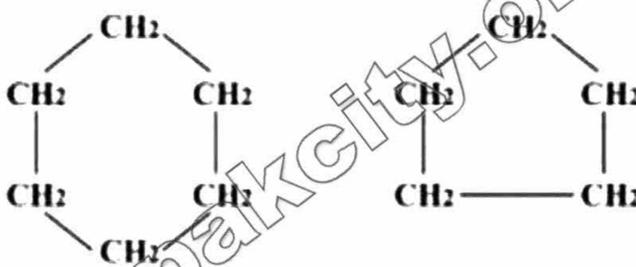
(3-Ethyl-2-methylhexane)



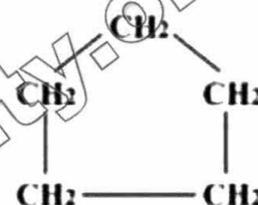
(2, 3, 5-Trimethylhexane)



(Cyclobutane)



(Cyclohexane)

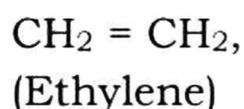


(Cyclopentane)

NOMENCLATURE OF ALKENES

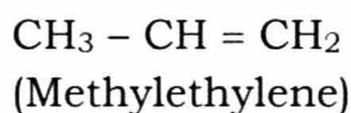
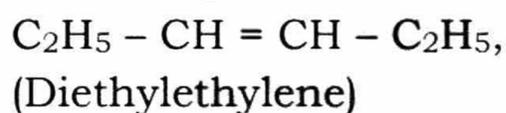
Common system

In common system, alkenes are named by replacing the suffix "ane" with "ylene" for example ethylene, propylene, butylene.



An alternative way of naming alkenes is by considering them as derivatives of ethylene.

For example

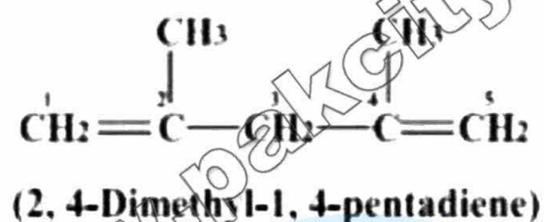
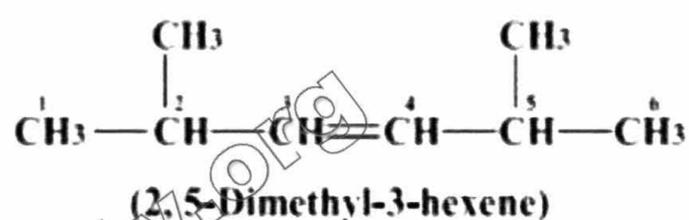
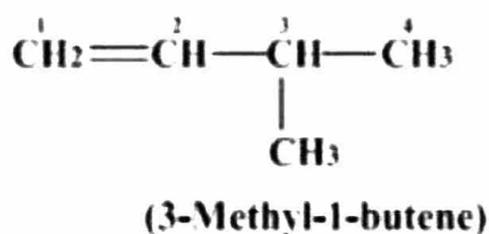


IUPAC System

In the IUPAC naming of alkene the suffix "ene" is used to indicate the presence of double bond.

Consider the following general rules as a guideline for naming alkene molecule according to IUPAC system.

- Select the longest carbon chain which must contain double bonded carbon atoms.
- The numbering of the longest chain starts from that end nearest to the carbon-carbon double bond irrespective of the location of alkyl radicals.
- Indicate the position of double bond by specifying the location of carbon atoms involved in the double bond.
- If there are more than one double bonds present within the carbon chain they are indicated by adding the prefixes di, tri etc. before the suffix "ene".

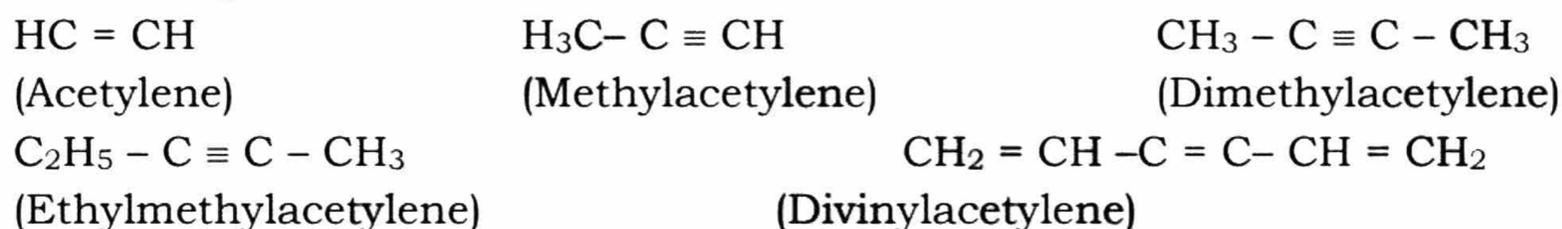


NOMENCLATURE OF ALKYNES

Common System

In common system, the first member of alkyne family is named as acetylene (C₂H₂). The name of higher alkynes are derived from acetylene by considering the branched carbon atoms as alkyl radicals.

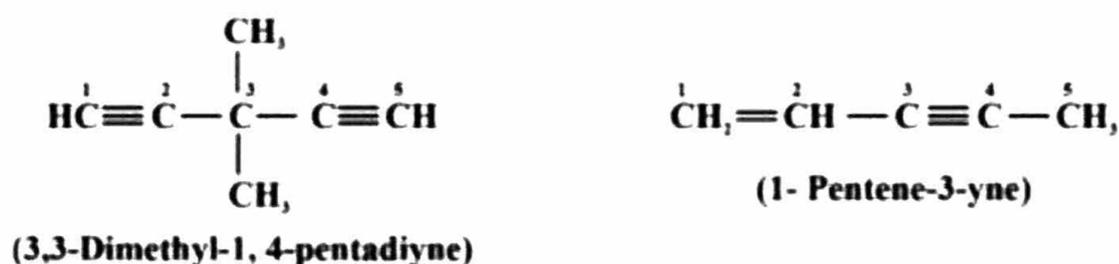
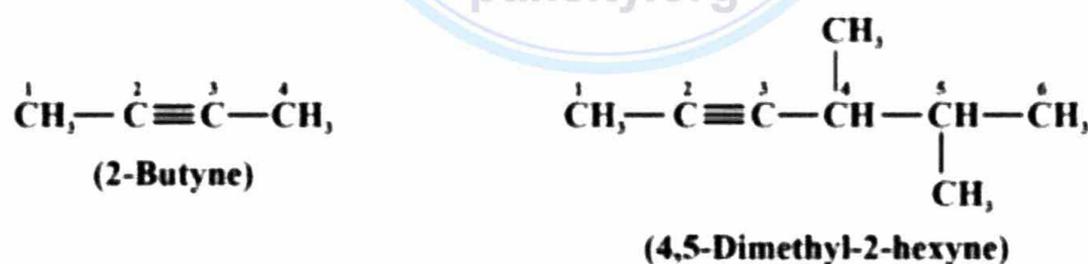
For example



IUPAC System

To write IUPAC names of alkynes, it is necessary to consider the following essential rules.

- a. Select the longest continuous carbon chain which must include both the carbon atoms containing triple bond.
- b. The numbering of carbon chain starts from the terminal which is nearest to the carbon-carbon triple bond.
- c. Write the name of parent alkanes for the same number of carbon atoms, replacing suffix "ane" with "yne" to indicate the presence of triple bond.
- d. Indicate the position of triple bond by specifying the location of the carbon atom involved in the bond.
- e. If two or more triple bond are present in the chain then they are indicated by adding the prefix di, tri etc. before the suffix -yne.
- f. When both double and triple bonds are present in the molecule at different positions then the numbering starts from the end where the bond (double or triple) is nearest.
- g. When double and triple bonds are present in the molecule at equal positions from the end, then the preference of numbering is given to double bond.

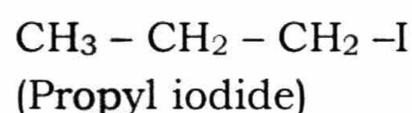
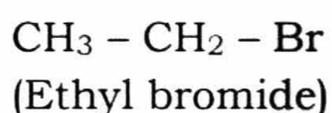
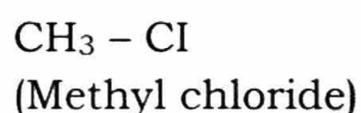


NOMENCLATURE OF ALKYL HALIDES

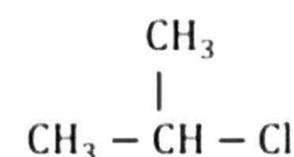
Alkyl halides are the derivatives of alkanes in which one or more hydrogen of alkanes are replaced by halogen atom.

Common System

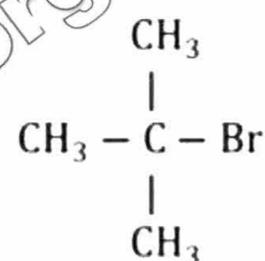
The common name of an alkyl halide is formed by naming the alkyl group first, followed by the term "halide".



The term secondary (sec.) and tertiary (tert.) are used as prefix if the carbon atom bonded to halogen is further attached to two and three other carbon atoms respectively.

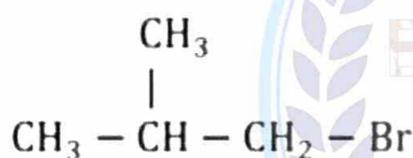


(sec-Propyl chloride)

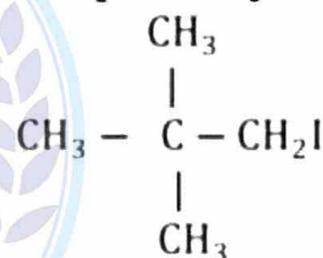


(tert-Butyl bromide)

The term iso and neo are also used as prefix when penultimate carbon is further attached to two or three other carbon atoms respectively.



(Isobutyl bromide)



(Neo pentyl iodide)

IUPAC System

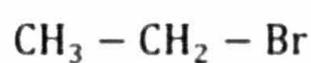
In IUPAC system alkyl halides are named as haloalkanes, where halo is chloro, bromo, iodo etc. When naming alkyl halides according to IUPAC system, it is important to adhere to the following rules.

- Determine the longest carbon chain that contains the carbon atom directly bonded to halogen.
- Number the carbon atoms in the chain from the end closest to the halogen atom.

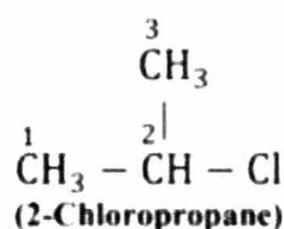


- c. When a double or triple bond is present in the halogenated carbon chain it is recommended to number the chain from the end nearest to the double or triple bond.
- d. Prefix di, tri, tetra etc. are used to indicate the number of halogens attached to the main carbon chain.
- e. When two different halogens are attached to the carbon chain at the same position from opposite ends, the halogen name will be written by its alphabetical order.

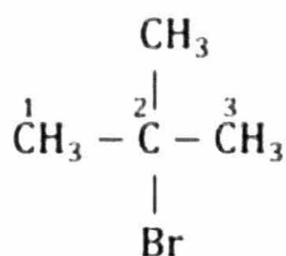
alphabetical order.



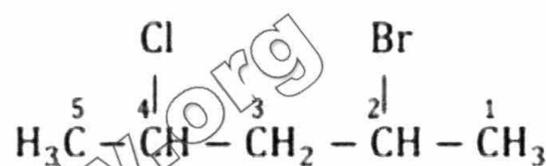
(Bromoethane)



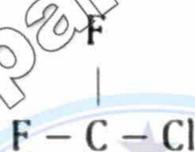
(2-Chloropropane)



(2-Bromo-2-methylpropane)



(2-Bromo-4-chloropentane)



(Dichlorodifluoromethane)

EDUCATION



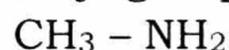
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NOMENCLATURE OF AMINES

Amines are organic compounds that contain a nitrogen atom bonded to one or more alkyl or aryl groups. Primary amines contains one alkyl group bonded to the nitrogen atom while secondary and tertiary amine are identified by the direct attachment of two and three alkyl groups with the nitrogen atom respectively.

Common System

The common name of a primary amine is formed by combining the name of alkyl group with the suffix "amine".

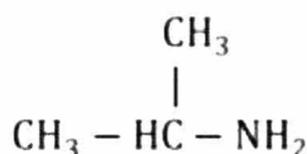


(Methyl amine)

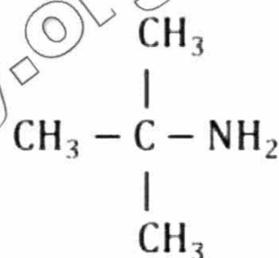


(Ethyl amine)

The prefix sec. and tert. are used if the carbon atom bonded to nitrogen is further attached with two or three alkyl radicals.



(sec-Propyl amine)

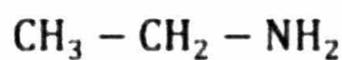


(tert-Butyl amine)

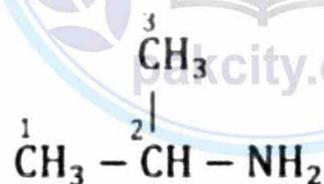
IUPAC System

In IUPAC system, primary amines are named as alkanamine and based on the following rules.

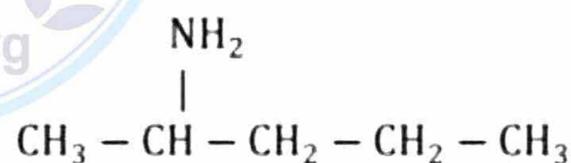
- 1) Select the longest carbon chain that contain the carbon atom directly bonded to $-\text{NH}_2$ group.
- 2) Write the name of compound by replacing the ending "e" of alkane chain by adding the suffix "amine".



(Ethanamine)



(2-Propanamine)



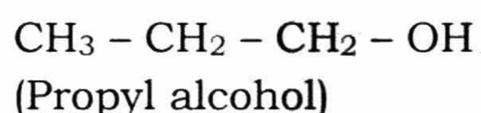
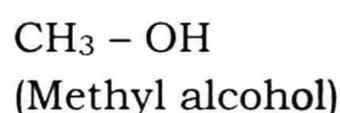
(2-Pentanamine)

NOMENCLATURE OF ALCOHOLS

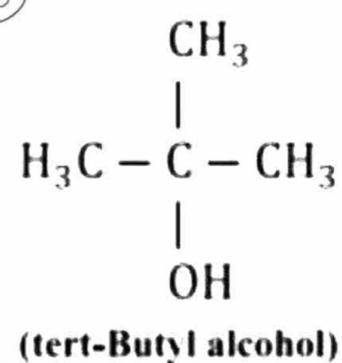
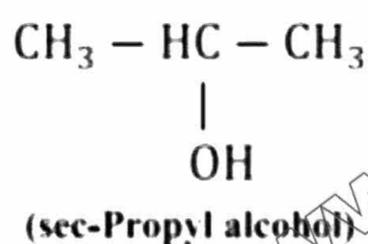
Organic compounds that contain one or more hydroxyl (-OH) functional group attached to the carbon chain are called alcohols.

Common System

Since alcohols are hydroxyl derivatives of hydrocarbons, their common names are formed by combining the name of alkyl group with the suffix "alcohol".



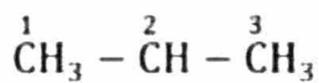
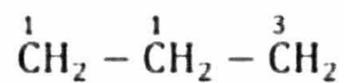
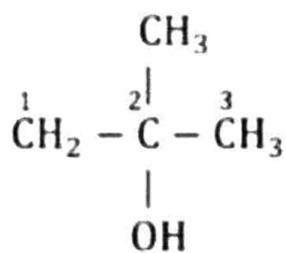
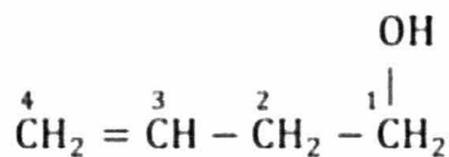
If the carbon atom bearing the hydroxyl group is directly connected to two or three other carbon atoms, the term secondary and tertiary is used as a prefix.



IUPAC System

The set of rules established by IUPAC system for the naming of alcohol is given as follow:

- Identify the longest continuous carbon chain that include the carbon atom bearing the hydroxyl group (-OH).
- Number the carbon atoms in the chain starting from the end nearest to the hydroxyl group.
- The end "e" of the parent alkane is replaced by "ol".
- If the molecule of alcohol has substituents (CH₃, Br, Cl, I etc), name them as prefixes.
- If two or more hydroxyl groups are present in the carbon chain, use di, tri etc. before the suffix -ol".
- The positions of substituents should be written in alphabetical order.

**(Ethanol)****(2-Propanol)****(1, 3-Propanediol)****(2-Methyl-2-propanol)****(3-Buten-1-ol)**

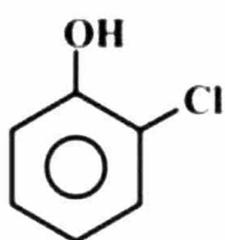
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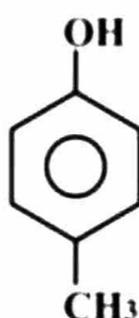
NOMENCLATURE OF PHENOLS

The class of organic compounds in which one or more hydroxyl group are directly attached with the benzene ring are called as phenols.

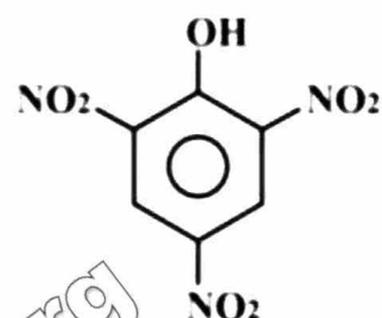
In the IUPAC nomenclature system, the parent molecule is referred phenol while numbering the substituents, the hydroxyl group (OH) is assigned the default first position. The term ortho, (-o), meta (-m) and para (-p) may be used for mentioning the position of substituents. It is important to note that certain phenols are still used by their trivial names in IUPAC system of nomenclature.



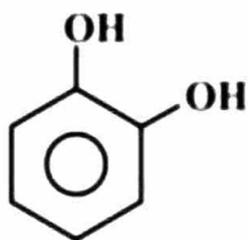
(2-Chlorophenol)
(o-Chlorophenol)



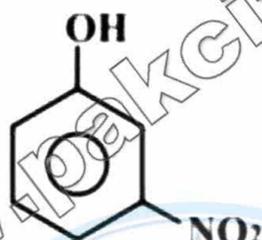
(4-Methylphenol)
(p-Cresol)



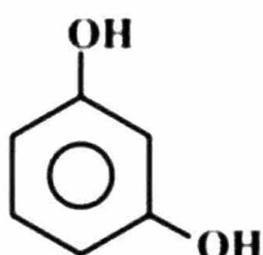
(2, 4, 6-Trinitrophenol)
(Picric acid)



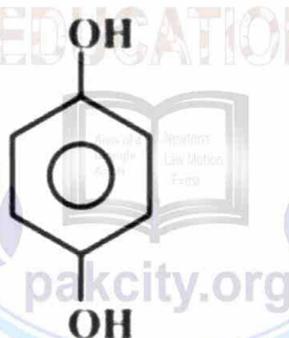
(1, 2-Benzenediol)
(Catechol)



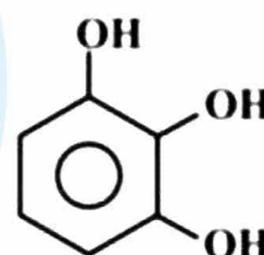
(3-Nitrophenol)
(m-Nitrophenol)



(1, 3-Benzenediol)
(Resorcinol)



(1, 4-Benzenediol)
(Hydroquinone)



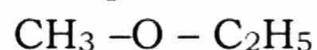
(1, 2, 3-Benzenetriol)
(Pyrogallol)

NOMENCLATURE OF ETHERS

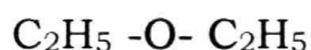
Ether is a family of organic compounds in which two alkyl or aryl radicals are attached to an oxygen atom. These compounds are represented by R-O-R.

Common System

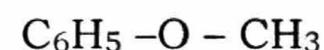
In the common system of naming of ethers, the two alkyl groups are written in alphabetical order and the term ether is added at the end of the name.



(Ethyl methyl ether)
ether)



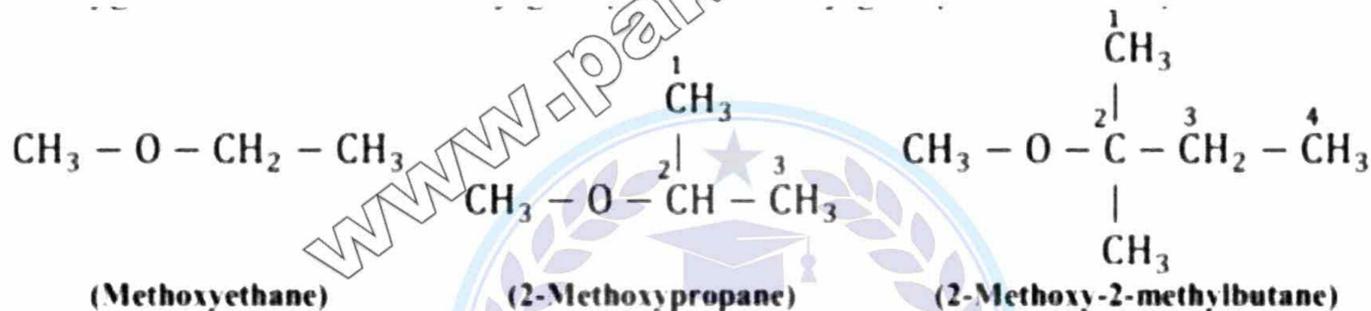
(Diethyl ether)



(Methyl phenyl ether)

IUPAC System

In IUPAC system of nomenclature, ethers are referred to as alkoxy derivatives of alkanes. The alkyl group of larger number of carbon atoms is considered as the main carbon chain whereas the smaller alkyl group, along with its oxygen is named as alkoxy group. The alkoxy group is taken as prefix.



NOMENCLATURE OF ALDEHYDES AND KETONES

Aldehydes and ketones are characterized by the presence of a carbonyl group. (C=O). Aldehydes have carbonyl group at the end of carbon chain whereas ketones have the carbonyl group within the carbon chain.

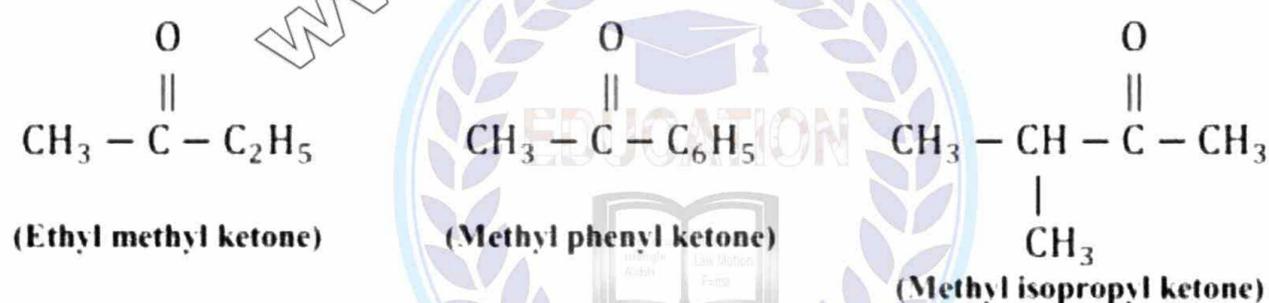
Common System

The common name of aldehyde is derived from the corresponding parent carboxylic acid by replacing -ic acid with the aldehyde.

For example

Parent Carboxylic Acid	Aldehyde
$\begin{array}{c} \text{O} \\ \\ \text{H} - \text{C} - \text{OH} \\ \text{(Formic acid)} \end{array}$	$\begin{array}{c} \text{O} \\ \\ \text{H} - \text{C} - \text{H} \\ \text{(Formaldehyde)} \end{array}$
$\begin{array}{c} \text{O} \\ \\ \text{CH}_3 - \text{C} - \text{OH} \\ \text{(Acetic acid)} \end{array}$	$\begin{array}{c} \text{O} \\ \\ \text{CH}_3 - \text{C} - \text{H} \\ \text{(Acetaldehyde)} \end{array}$

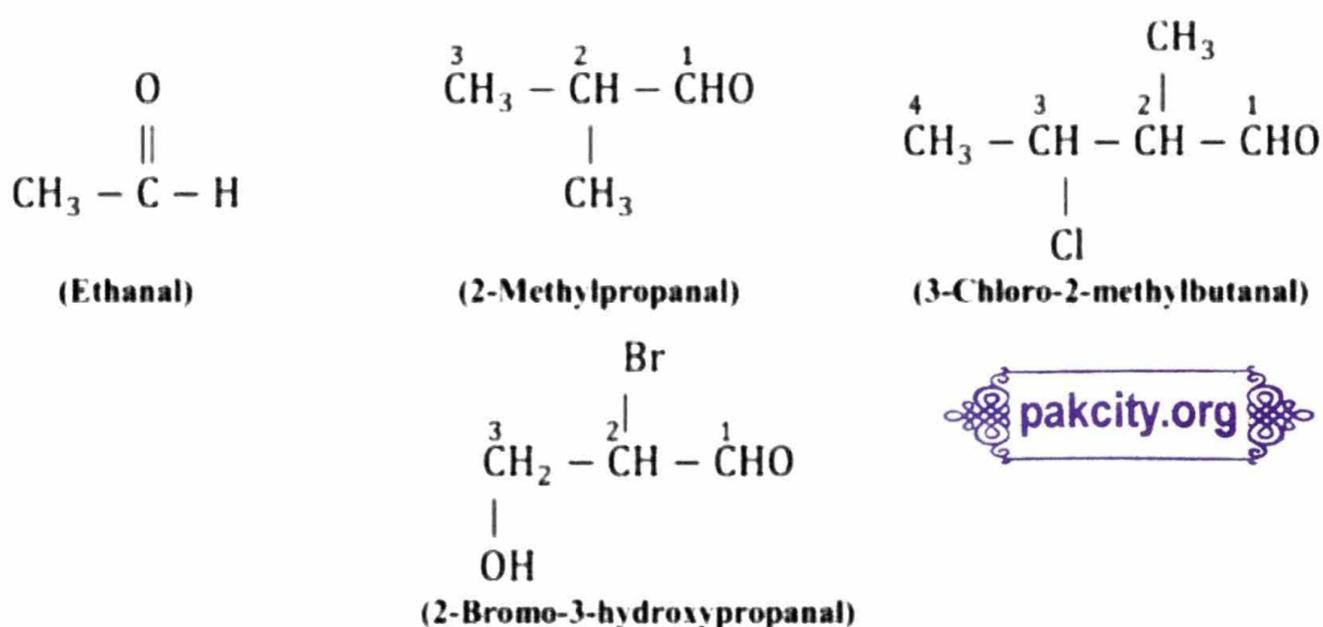
The common naming system of ketones is quite similar to that of ether. The two alkyl groups attached to the carbonyl carbon are named in alphabetical order and the term ketone is added at the end of the name.



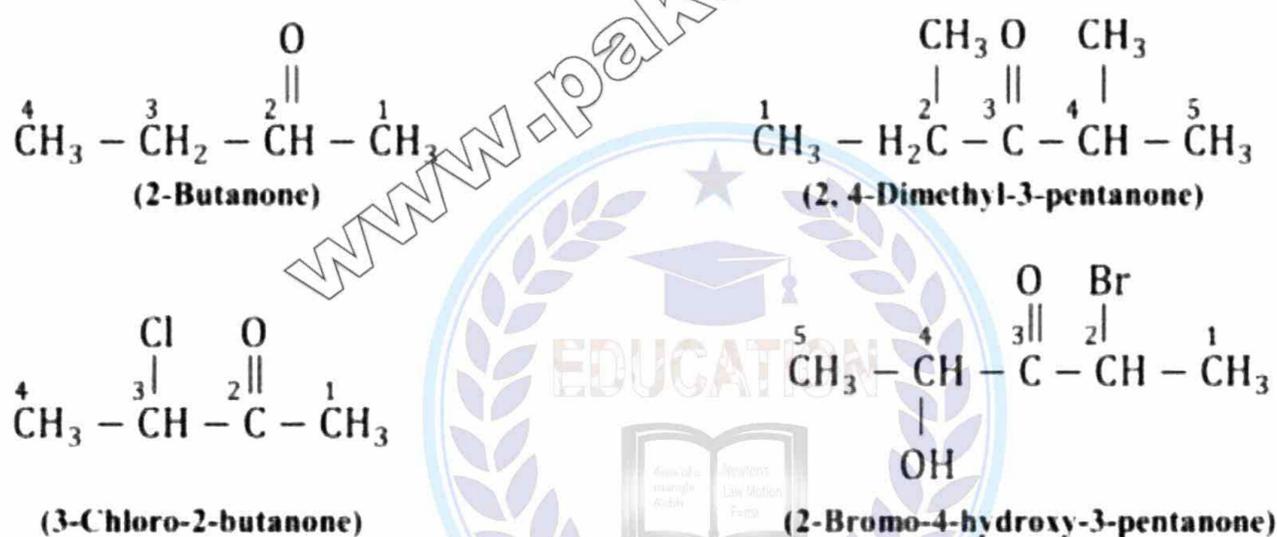
IUPAC System

In this system aldehydes are named after the name of corresponding alkanes. The ending "e" of alkane being replaced by suffix -al. The longest carbon chain containing the CHO group is chosen as the parent chain. The position of substituents are indicated by the numbers of carbon atoms to which they are attached and the carbon atom of the -CHO group is given number one.

The hydroxyl group take preference over double bond and double bond take preference over halogens and alkyl groups if present in the molecule.



In the IUPAC naming of ketones, the longest carbon chain having the ketonic functional group is chosen as the parent chain and the ketone is named by replacing "-e" of the parent alkane with the suffix "one". The position of substituents are indicated by numbers of the carbon atoms to which they are attached and the carbon of carbonyl group is given the lowest possible number.



NOMENCLATURE OF CARBOXYLIC ACIDS

Organic compounds which contain carboxyl group ($-\text{COOH}$) are known as carboxylic acids.

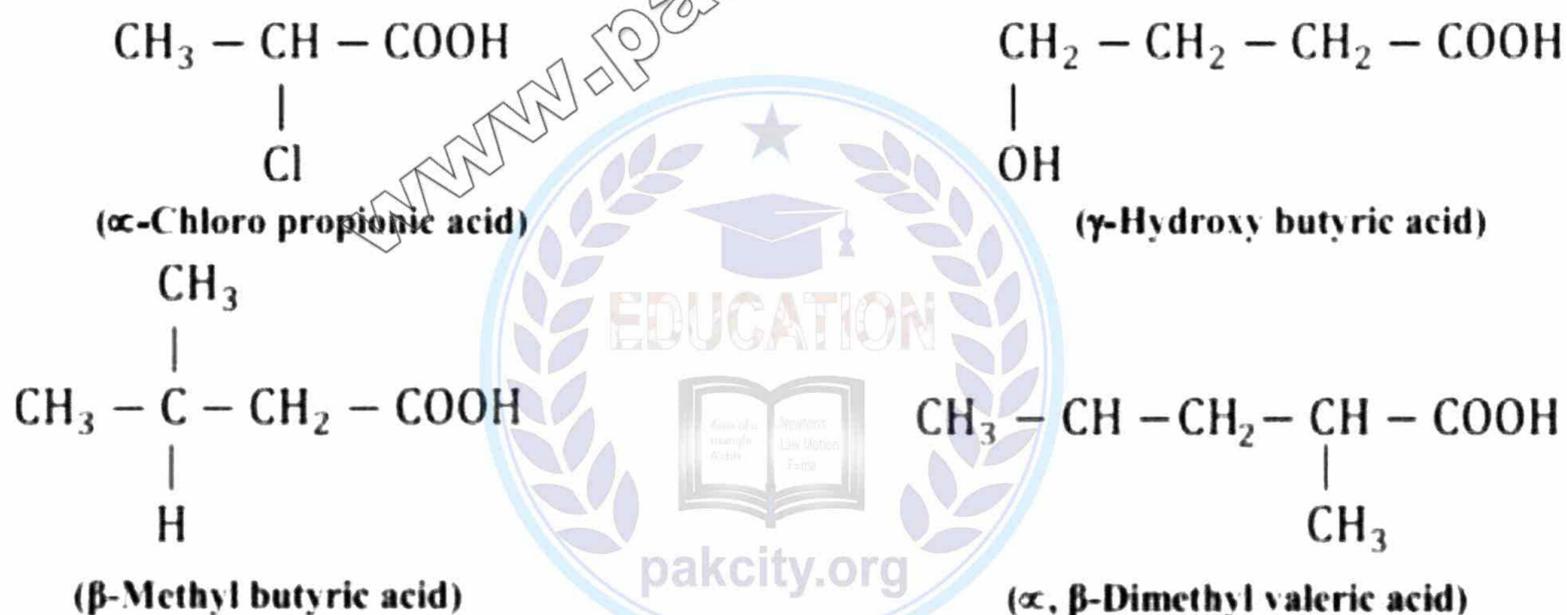
Common System

The common names of mono carboxylic acids refers to their sources rather than their chemical structures. Positions of substituents is designated by, B and Y etc.

Common names of some carboxylic acids are given below.

Structure	Common name
HCOOH	Formic acid
CH ₃ COOH	Acetic acid
CH ₃ CH ₂ COOH	Propionic acid
CH ₃ (CH) ₂ COOH	Butyric acid
CH ₃ (CH ₂) ₂ COOH	Valeric acid
CH ₃ (CH ₂) ₄ COOH	Caproic acid

Common names of carboxylic acid are given as

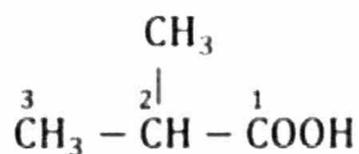


IUPAC System

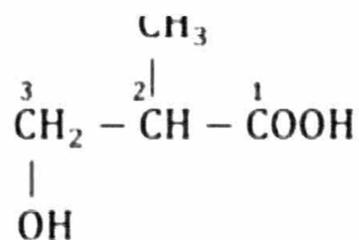
The name of carboxylic acid in IUPAC system is referred as alkanonic acid. The longest continuous carbon chain containing the $-\text{COOH}$ group is considered the parent chain and the acid is named by replacing -e of the corresponding alkane with "oic acid".

Double bond in the main chain are written by the ending -enoic acid and its position is designated by numerical prefix. When two $-\text{COOH}$ groups are present in the main chain, use the prefix 'di' before the suffix oic acid. When

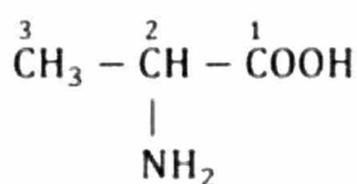
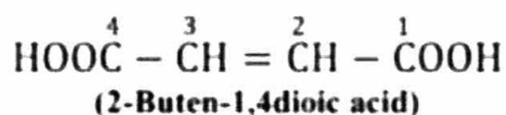
a carboxylic acid is attached to benzene ring the parent ring, named as benzoic acid.



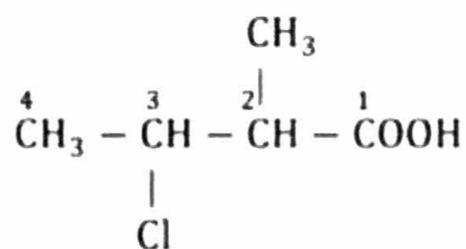
(2-Methyl propanoic acid)



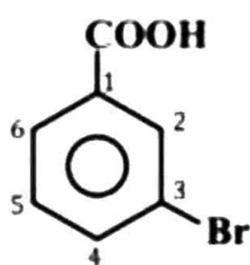
(3-Hydroxy-2-methyl propanoic acid)



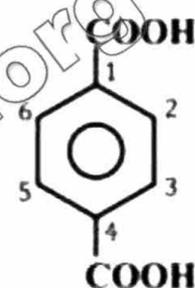
(2-Aminopropanoic acid)



(3-Chloro-2-methylbutanoic acid)



(3-Bromobenzoic acid)



(Benzen-1, 4-dioic acid)



NOMENCLATURE OF ESTERS

Esters are named as alkyl derivatives carboxylic acids. Following steps should be noted for the naming of ester molecules.

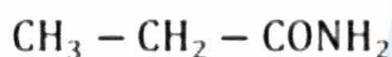
- 1) Find the longest carbon chain which contains -COO- group.
- 2) Write the name of alkyl group which is attached to R-COO- chain.
- 3) Name the carbon chain that contain ester functional group using "oate" as a suffix.

Common system of nomenclature of ester is quite similar with IUPAC method. Here "ate" is used as suffix with the main carbon chain.

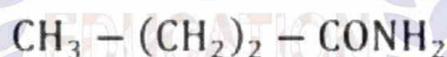
Structure of Ester	Common Name	IUPAC Name
HCOOC ₂ H ₅	Ethyl formate	Ethyl methanoate
CH ₃ - CH ₂ -COO- CH ₃	Methyl propionate	Methyl propanoate
CH ₃ (CH ₂) ₂ COOC ₂ H ₅	Ethyl butyrate	Ethyl butanoate
CH ₃ COOCH(CH ₃) ₂	Isopropyl acetate	Isopropyl ethanoate

NOMENCLATURE OF AMIDE

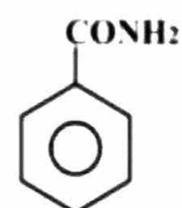
Amides are the derivate of carboxylic acids formed by replacing -OH group of carboxylic acid by NH₂ group. The nomenclature of amide is based on replacing the suffix -oic acid with amide. For example



(Propanamide)



(Butanamide)



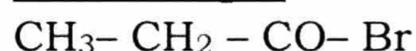
(Benzamide)

NOMENCLATURE OF ACYL HALIDES

Acyl halides or acid halides are derived from carboxylic acids. They are characterized by the presence of a halogen atom attached to acyl group (R-CO-).

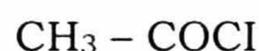
When naming an acyl halide, the work begins with the name of the corresponding carboxylic acid. In both common and IUPAC method the ic acid ending the carboxylic acid is replaced by -yl, and then name the specific halide group.

For example



Propanoyl bromide (IUPAC)

Propionyl bromide (common)



Ethanoyl chloride (IUPAC)

Acetyl chloride (common)

Short Questions

1. Why IUPAC system of nomenclature is preferred on common system of naming of organic compounds?

The IUPAC system of nomenclature for organic compounds is preferred over the common system of naming for several reasons:

- Unambiguousness: The IUPAC system provides a unique and unambiguous name for every organic compound, regardless of its complexity. This is because the name is based on the structure of the compound, rather than on any arbitrary or historical criteria.
- Systematic: The IUPAC system is a systematic approach to naming organic compounds. This means that there are a set of rules that can be followed to generate a name for any compound. This makes it easy to learn and apply the system.
- International: The IUPAC system is an internationally accepted standard for naming organic compounds. This means that chemists from all over the world can communicate with each other using the same nomenclature system.



2. Write the name of five organic families and mention the functional group present in them.

Family	Functional group
Alkanes	Alkyl group (C–C)
Alkenes	Carbon-carbon double bond (C = C)
Alkynes	Carbon-carbon triple bond (C ≡ C)
Alcohols	Hydroxyl group (– OH)
Carboxylic acids	Carboxyl group (– COOH)

3. Write down basic rules for IUPAC naming of organic compound.

Notes Pg #

4. We often use the term Iso and Neo in the common system of naming of alkanes. Explain with example

The terms "iso" and "neo" are used in the common system of naming alkanes to indicate specific branching patterns.

- Iso: The prefix "iso" is used to indicate that the compound is a branched alkane with a methyl group attached to the second carbon atom. For

example, isobutane is a branched alkane with a methyl group attached to the second carbon atom of a three-carbon chain.

- Neo: The prefix "neo" is used to indicate that the compound is a branched alkane with a tertiary butyl group attached to a carbon atom. For example, neopentane is a branched alkane with a tertiary butyl group attached to the second carbon atom of a three-carbon chain.

Here are some more examples:

Compound	Common name	IUPAC name
$\text{CH}_3\text{CH}(\text{CH}_3)_2$	Isobutane	2-Methylpropane
$(\text{CH}_3)_3\text{CH}$	Neopentane	2,2-Dimethylpropane
$(\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3))_2$	Isoheptane	2-Methylhexane
$(\text{CH}_3)_3\text{CCH}_2(\text{CH}_3)_3$	Neooctane	2,2,4-Trimethylpentane

5. Write the common names of first five members of carboxylic acid.

The common names of the first five members of the carboxylic acid family are:

- Formic acid (HCO_2H)
- Acetic acid (CH_3COOH)
- Propionic acid ($\text{CH}_3\text{CH}_2\text{COOH}$)
- Butyric acid ($\text{CH}_3(\text{CH}_2)_2\text{COOH}$)
- Valeric acid ($\text{CH}_3(\text{CH}_2)_3\text{COOH}$)

6. If an organic compound contains both double and triple bond, in the main carbon chain, what rules you follow to write its IUPAC name.

Explain by giving an example.

When naming an organic compound that contains both a double and a triple bond in the main carbon chain, the following rules are followed:

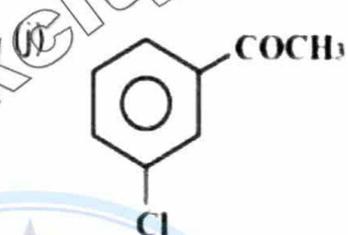
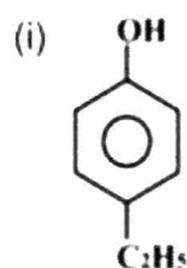
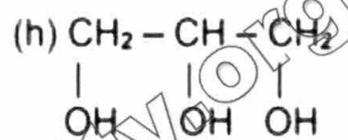
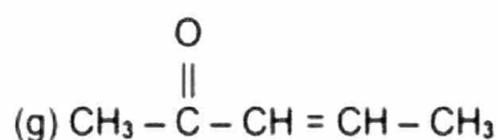
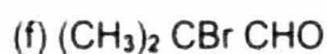
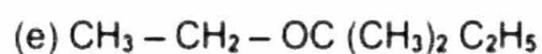
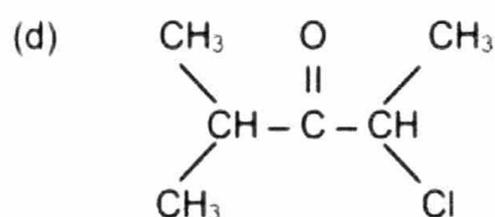
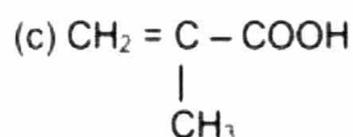
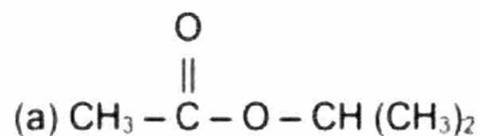
1. Choose the longest carbon chain that contains both the double and triple bond.
2. Number the carbon atoms in the longest chain, starting from the end that is closest to the multiple bonds.
3. If the double and triple bonds have the same number, the double bond is given the lower number.
4. The suffixes "-ene" and "-yne" are added to the end of the parent chain name, in that order.
5. The numbers of the carbon atoms where the double and triple bonds occur are placed in front of the suffixes, and separated by a hyphen.

Example:

The IUPAC name of the compound $\text{CH}_3 - \text{CH} = \text{CH} - \text{C} \equiv \text{C}$ is: **2-buten-4-yne**

Descriptive Questions

1. Give the IUPAC names of the following organic molecules.



2. Outline the structure of each of the following molecules.

(a) Ethyl neo-pentyl ether (b) Resorcinol

(c) Picric acid (d) Isopropylbutanoate

(e) 1-Bromo-3-methyl hexane-2-one (f) α , β -dimethyl butyric acid

(g) Butyraldehyde (h) 3-Chlorobenzamide

(i) Butanoyl iodide (j) 1, 2,3-benzentriol

(k) Ethyl isopropyl ketone (l) β -Methyl butyraldehyde

(m) β -Chloro- β -methyl valeric acid