# 3.1.IUPAC Nomenclature of Organic Molecules

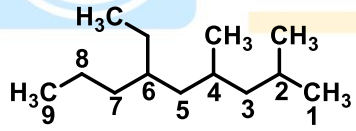
## *3.1.1. IUPAC*

- The International Union of Pure and Applied Chemistry (IUPAC) system of naming is primarily based on (a) Word root, (b) Suffix and (c) Prefix.
- **Word root**: It is the number of carbon atoms present in the longest chain of the compound.
- **Suffix**: Primary suffix indicates the number of unsaturation in the carbon chain. Secondary suffix indicates the functional group present in the organic compound.
- **Prefix**: In case of cyclic compounds, the primary prefix, cyclo is added before the word root of the parent chain of the compound.

❖ **General Rules for IUPAC Nomenclature of Organic Compounds**

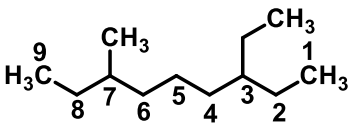
- **Nomenclature of Saturated Hydrocarbons (Alkanes)**

1. Selection of longest carbon chain which is called parent chain.
2. Number of the carbon atoms in the parent chain as 1,2,3….etc.,When two or more substituents attached to the parent chain, then lowest set of locants is preferred for numbering.
3. If two or more substituent are present on the parent chain, they appeared in the alphabetical order.



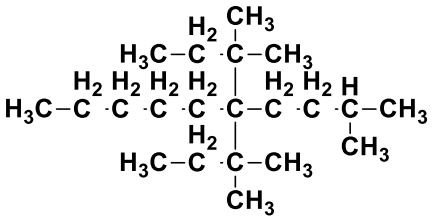

6-ethyl-2,4-dimethyl nonane
(not 2,4-dimethyl-6-ethylnonane)

4. When two different alkyl locants are present at the equal distance from the two ends of the main chain, the numbering will be in the alphabetical order.



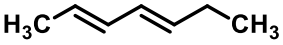

3-ethyl-7-methylnonane
(not 3-methyl-7-ethylnonane)

Note: When the two same complex substituent occur more than once, it is indicated by multiplying prefix bis, tris, tetrakis etc.



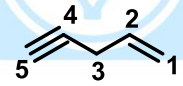
5,5-bis (1,1-dimethylpropyl) 2-methyldecane

- **Nomenclature of Unsaturated Hydrocarbons (Alkenes and Alkynes)**
- 1. The multiple bond must be longest chain.
- 2. The suffix "ane" of the corresponding alkane is replaced by "ene" and "yne" for double and triple bond.
- 3. If a compound contains two or more multiple bonds, the letter "a" should be added to word root.



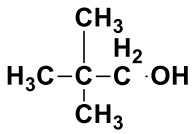
2,4-heptadiene

- 4. The numbering of atoms in the parent chain is done in such a way that the multiple bonds (doble or triple bonds) gets the lowest number.
- 5. When there is a choice of numbering between double or triple bond, the double bonds are given lowest number.

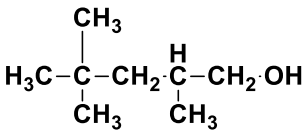


1-penten-4-yne

- **Nomenclature of Compounds Having Functional Group**
  1. The longest chain containing the carbon atom having functional group must be selected first.
  2. The numbering of the atoms in the parent chain is done in such a way that the carbon atom having the functional group will get the lowest number.



2,2-dimethylpropan 1-ol

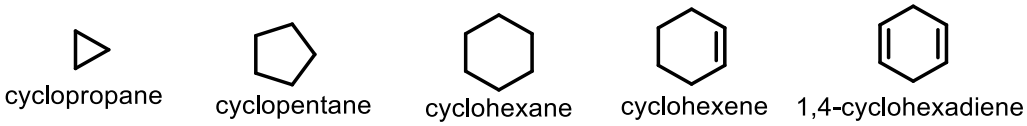


2,4,4-trimethylpentan-1-ol

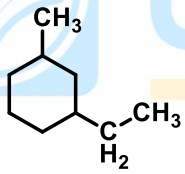
3. The functional group such as –CHO, -COOH, -CONH2, -CN etc always starts the numbering of the parent chain.
4. If a compound contains several functional groups, the senior most functional group will be considered as a principal functional group (suffix) while all other will be treated as prefix.
5. The other groups like halo, nitro, nitroso, and alkoxy are always treated as substituent groups.

- **Nomenclature of Compounds Alicyclic Compounds**

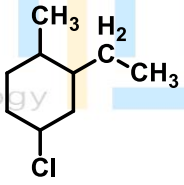
1. The name of the alicyclic compounds is determined by adding prefix "cyclo" to the name of the compound (alkane, alkene and alkyne).




2. If only one substituent is present, then it is not needed to indicate its position; however, if two or more substituent are present in the ring, their position must be designated by arabic numerical (1,2,3,4…etc) and in alphabetical order.

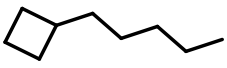



1-ethyl-3-methylcyclohexane
(not 1-ethyl-5-methylcyclohexane)




4-chloro-2-ethyl-1-methylcyclohexane
(not 1-chloro-3-ethyl-4-methylcyclohexane)

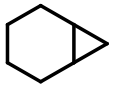
3. When a single ring is attached to a single chain with a greater number of carbon atoms or when more than one ring system is attached to a single chain, then the naming will be as cycloalkylalkane.



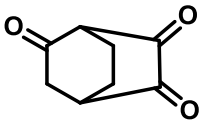
1-cyclobutylpentane

1,3-dicyclohexylpropane

- **Nomenclature of Bicyclic Compounds**
  1. Cycloalkanes containing two rings only and having two or more atoms in common are named by adding prefix bicycle followed by the name of the alkane. Inbetween bicycle and alkane, number of carbon atoms representing the bridge are written within the bracket.

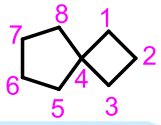


Bicyclo [4,1,0] heptane

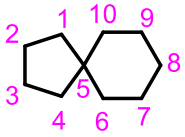



Bicyclo [2,2,2] octane 2,3,5-trione

- **Nomenclature of Spiro Compounds**
  1. Two rings with one common atom is called spiro ring system

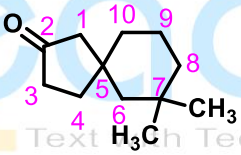



Spiro[3,4] octane




Spiro[4,5] decane


Spiro[3,4] oct-5-ene

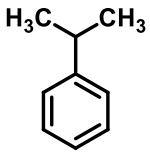



7,7-dimethylspiro[4,5] dec-2-one

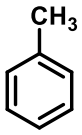
- **IUPAC Nomenclature of Aromatic Compounds**

The following compounds can be named as follows…….

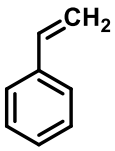
Benzene



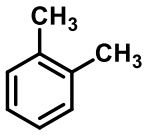

Cumene



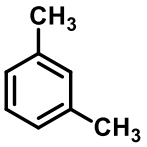

Toluene



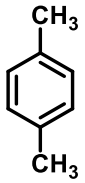

Styrene



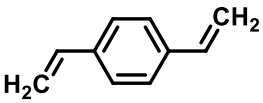

*o*-xylene



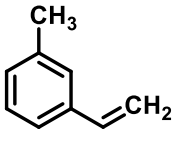

*m*-xylene



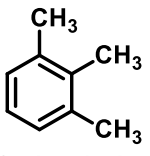

*p*-xylene




1,4-divinyl benzene

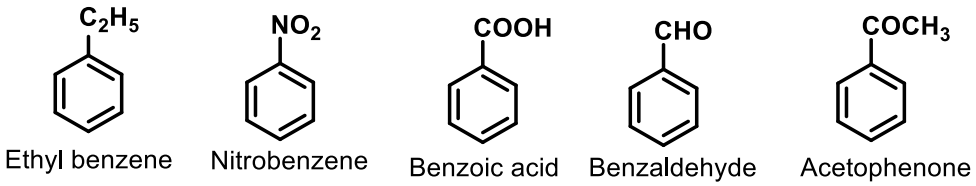



1-methyl-3-vinyl benzene

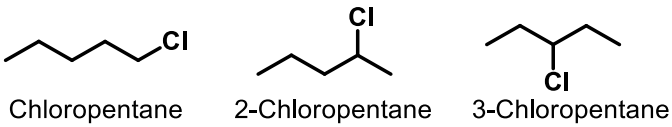



1,2,3-trimethylbenzene

- **Benzene derivatives**:




- **IUPAC Nomenclature of Regioisomers**




- ***R, S*-Nomenclature for Stereoisomers**

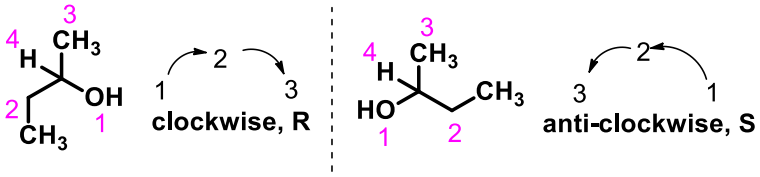
The different stereoisomers of a molecule can be expressed in terms of *R* and *S* configuration. This method was proposed by Cahn, Ingold and Prelog (CIP). This method involves the following steps

Step I: Identification of centre of chirality in the molecule.

Step II: The four atoms or group of atoms joined to the asymmetric centre are assigned as sequence of the priority by the sequence rules. These are governed by CIP rule which suggests that (a) the four substituent are listed decreasing order of atomic number, (b) If the relative priority of two groups is not decided by **rule a**, then the next atoms must be considered for priority assignment.

Step III: After assigning the priorities of the four groups or atoms attached to the asymmetric carbon atom the molecule is visualized in a position where the atom or group of atoms of lowest priority is directed away from us.

- If the sequence is left to right, i.e. clockwise, then it will be R (R stands for **rectus** which is a Latin word for right)
- If the sequence is right to left, i.e. anticlockwise, then it will be S (S stands for **sinister** which is a Latin word for left).

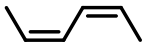


- ***E-Z* System of Nomenclature for Geometrical Isomers**

CIP developed the E-Z system which is based on the assignment of priorities of atoms or groups attached with each carbon of the double bond.

If the two higher priority groups are on the same side of the double bond, the isomer is called Z and if the two higher priority groups are on the opposite side of the double bond, then the isomer will be called E.

(Z)-3-hexene



(2Z, 4Z)-2,4-hexadiene