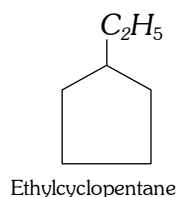
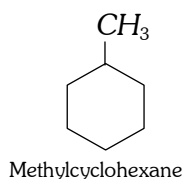
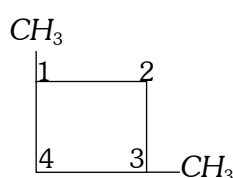




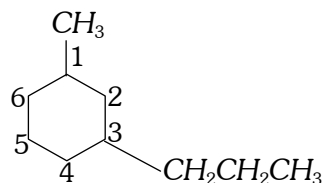
## Purification, classification and nomenclature of organic compound Part 2



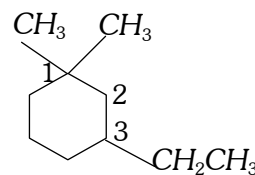
When more than one side chains are present, the numbering is done beginning with one side chain so that the next side chain gets the lower possible number. For example,



1,3-Dimethylcyclobutane

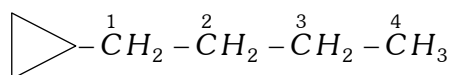


1-Methyl-3-propylcyclohexane  
(Not 5-Methyl-1-propyl cycloalkane)

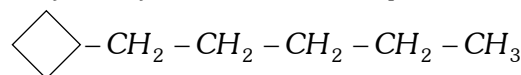


3-Ethyl-1,1-dimethylcyclohexane  
(Not 1-Ethyl-3,3-dimethylcyclohexane)

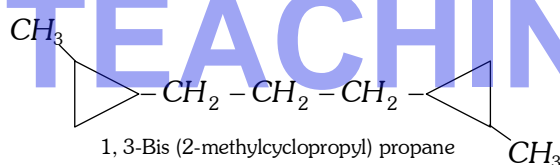
When a single ring system is attached to a single chain with a greater number of carbon atoms or when more than one ring system is attached to a single chain, then it is named as cycloalkylalkanes. For example,



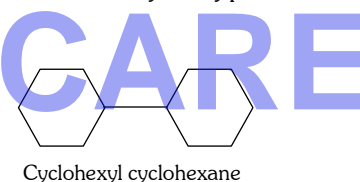
1-Cyclopropyl butane



1-Cyclobutylpentane

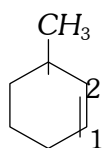


1,3-Bis(2-methylcyclopropyl) propane

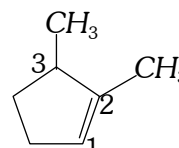


Cyclohexyl cyclohexane

In case of substituted cycloalkenes, the double bond is given the lowest possible number and numbering is done in such a way that the substituents get the lowest number.



3-Methylcyclohex-1-ene



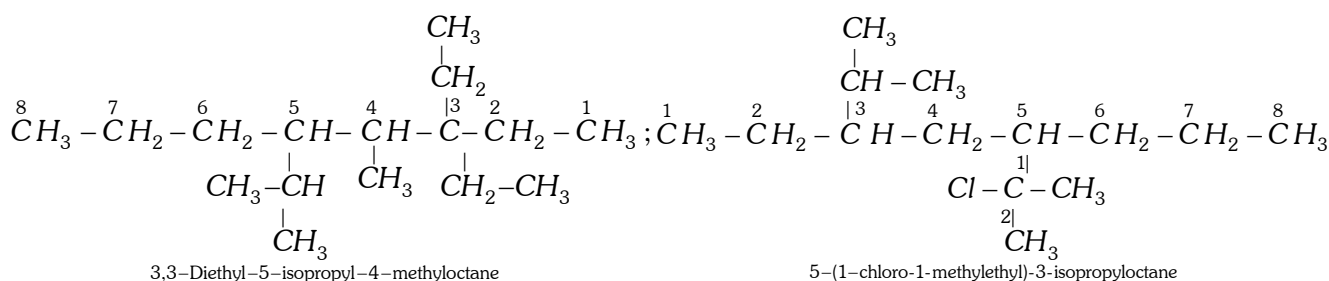
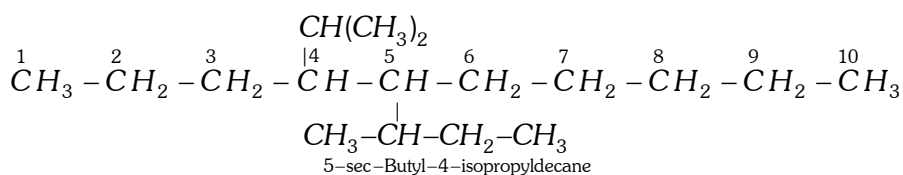
2,3-Dimethylcyclopent-1-ene

**Note :** According to the IUPAC system of Nomenclature, certain trivial or semi-systematic names may be used for unsubstituted radicals. For example, the following names may be used,

$(\text{CH}_3)_2\text{CH} -$	<b>Isopropyl</b>	$(\text{CH}_3)_2\text{CH} - \text{CH}_2 -$	<b>Isobutyl</b>
$\text{CH}_3 - \text{CH}_2 - \underset{\text{CH}_3}{\text{CH}} -$	<b>Sec-Butyl</b>	$(\text{CH}_3)_3\text{C} -$	<b>tert-Butyl</b>
$(\text{CH}_3)_2\text{CH} - \text{CH}_2 - \text{CH}_2 -$	<b>Isopentyl</b>	$(\text{CH}_3)_3\text{C} - \text{CH}_2 -$	<b>Neopentyl</b>
$\text{CH}_3 - \text{CH}_2 - \underset{\text{CH}_3}{\overset{\text{CH}_3}{\text{C}}} -$	<b>tert-Pentyl</b>	$(\text{CH}_3)_2\text{CH} - \text{CH}_2 - \text{CH}_2 - \text{CH} -$	<b>Isohexyl</b>

## Purification, classification and nomenclature of organic compound Part 2

However, when these are substituted, these names cannot be used as such. For example,



It may be noted that while writing the substituent's name in alphabetical order, the prefixes *iso*- and *neo*- are considered to be part of the fundamental name. However, the prefixes *sec*- and *tert*- are not considered to be the part of the fundamental name.

### (2) Rules for IUPAC names of polyfunctional organic compounds

Organic compounds which contain two or more functional groups are called polyfunctional compounds. Their IUPAC names are obtained as follows,

(i) **Principal functional group**: If the organic compound contains two or more functional groups, one of the functional groups is selected as the principal functional group while all the remaining functional groups (also called the secondary functional groups) are treated as substituents. The following order of preference is used while selecting the principal functional group.

*Sulphonic acids > carboxylic acids > anhydrides > esters > acid chlorides > acid amides > nitriles > aldehydes > ketones > thiols > alcohols > alkenes > alkynes.*

All the remaining functional groups such as halo (fluoro, chloro, bromo, iodo), nitroso (–NO), –nitro (–NO<sub>2</sub>), amino (–NH<sub>2</sub>) and alkoxy (–OR) are treated as substituents.

#### The decreasing order of seniority among the principal groups

Order of preference	Prefix	Suffix (ending)	Order of preference	Prefix	Suffix (ending)
– SO <sub>3</sub> H	Sulpho	Sulphonic acid	– OH	Hydroxy	– ol
– COOH	Carboxy	– oic acid	– NH <sub>2</sub>	Amine	– amine
– COOR	Alkoxy	Alkyl alkanoate	C = C	–	– ene
– COX	Haloformyl	Oyl halide	– C ≡ C –	–	– yne
– CONH <sub>2</sub>	Carbamoyl	– amide	– O –	Epoxy	–
– C ≡ N	Cyano	– nitrile	– X	Halo	–
– CHO	Formyl	– al	– NO <sub>2</sub>	Nitro	–
> C = O	Keto	– one			

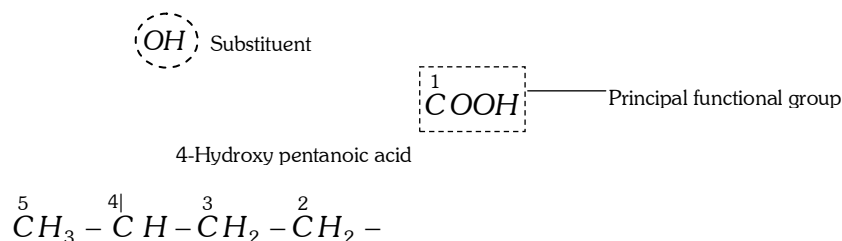
(ii) **Selecting the principal chain**: Select the longest continuous chain of carbon atoms containing the principal functional group and maximum number of secondary functional groups and multiple bonds, if any.

(iii) **Numbering the principal chain**: Number the principal chain in such a way that the principal functional group gets the lowest possible number followed by double bond and triple bond and the substituents, *i.e.*

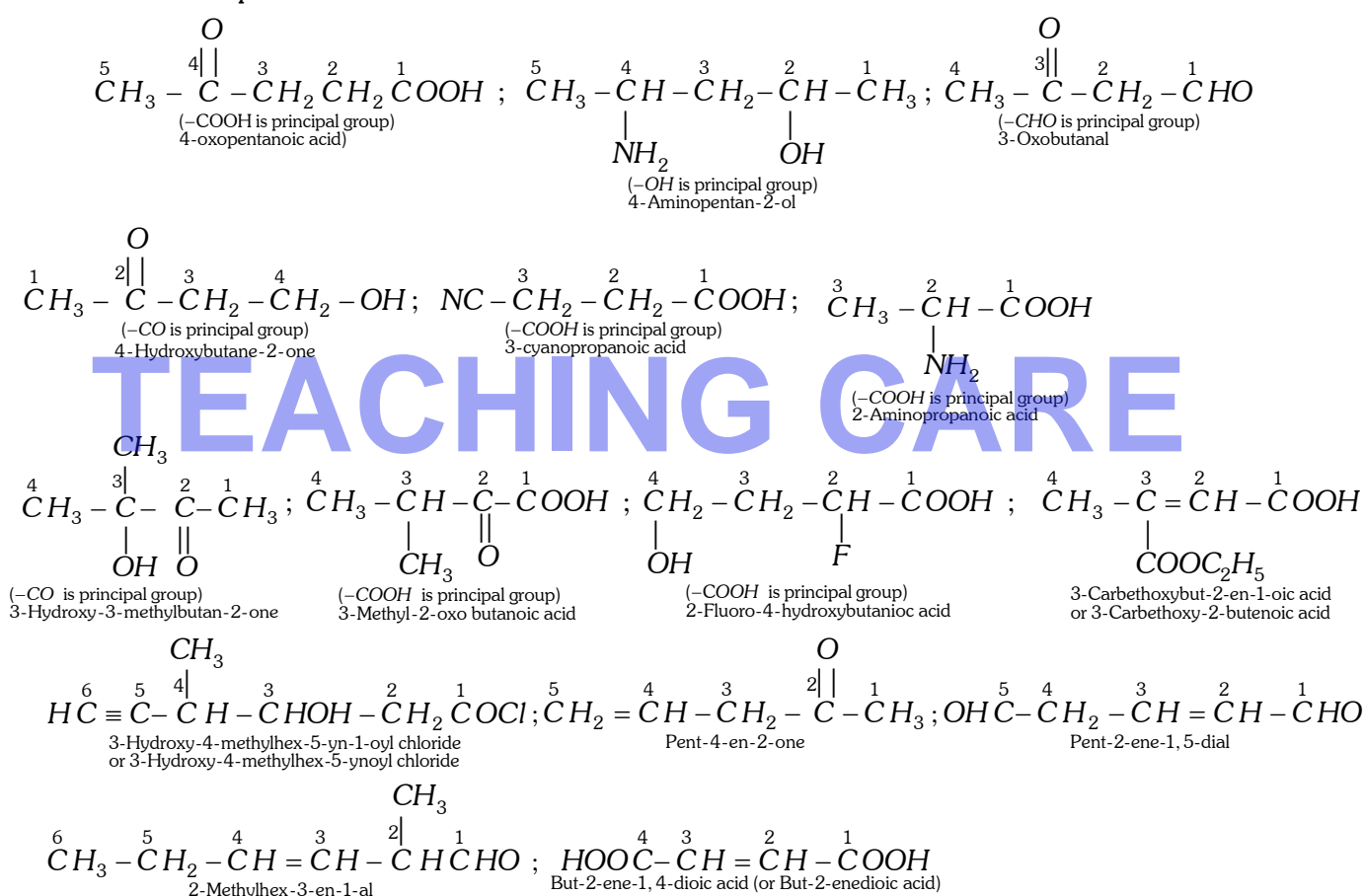
Principal functional group > double bond > triple bond > substituents

## Purification, classification and nomenclature of organic compound Part 2

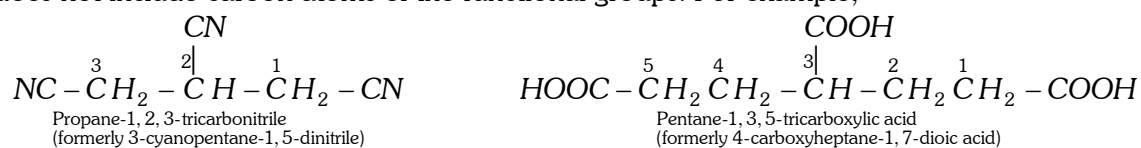
(iv) **Alphabetical order** : Identify the prefixes and the positional numbers (also called locants) for the secondary functional groups and other substituents and place them in alphabetical order before the word root.



Some other examples are :

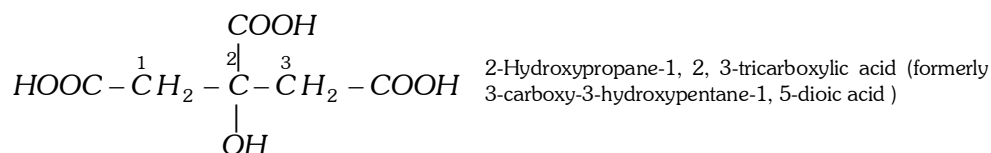


**(3) Polyfunctional compounds containing more than two like functional groups** : According to latest convention (1993 recommendations for IUPAC nomenclature), if an unbranched carbon chain is directly linked to more than two like functional groups, the organic compound is named as a derivative of the parent alkane which does not include carbon atoms of the functional groups. For example,

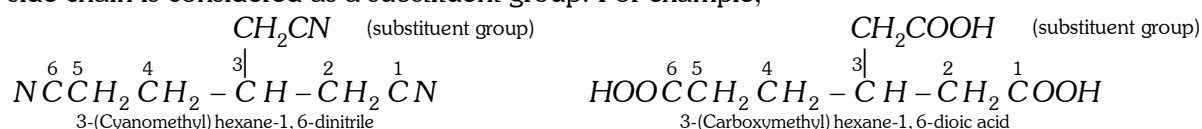


Following the above rule, citric acid may be named as,

## Purification, classification and nomenclature of organic compound Part 2

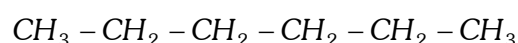


**Note** : \*If none of the choices in a multiple choice question follows 1993 recommendations, the choice corresponding to earlier system of nomenclature as given in parentheses should be taken as correct. If, however, all the three like groups are not directly linked to the unbranched carbon chain, the carbon atoms of the two like groups are included in the parent chain while the third which forms the side chain is considered as a substituent group. For example,



### Bond-line Notation of organic compounds

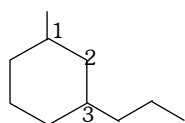
Sometimes, the bonds between carbon atoms are represented by lines. For example, *n*-hexane has a continuous chain of six carbon atoms which may be represented as,



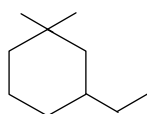
*n*-Hexane



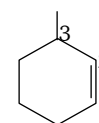
In this notation, the carbon atoms are represented by line ends and intersections. It is assumed that the required number of hydrogen atoms are present wherever they are necessary to satisfy the tetravalency of carbon. A single line represents a single bond (C – C), two parallel lines represent a double bond (C = C) and three parallel lines represent a triple bond (C ≡ C). For example,



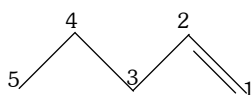
1-Methyl-3-propylcyclohexane



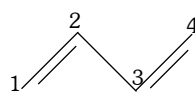
3-Ethyl-1, 1-dimethylcyclohexane  
(Not 1-ethyl-3, 3-dimethylcyclohexane)



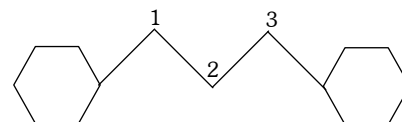
3-Methyl cyclohex-1-ene



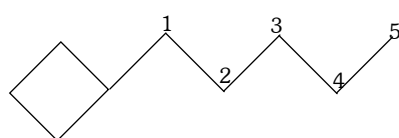
Pent-1-ene



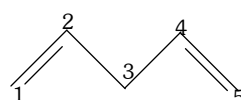
Buta-1, 3-diene



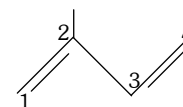
1,3-Dicyclohexyl propane



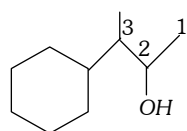
1-Cyclobutyl pentane



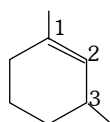
Penta-1, 4-diene



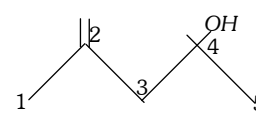
2-Methylbuta-1, 3-diene (a line at position 2 corresponds to CH<sub>3</sub> group)



3-Cyclohexyl butan-2-ol

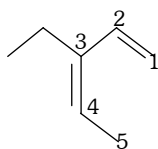


1, 3-Dimethyl cyclohex-1-ene

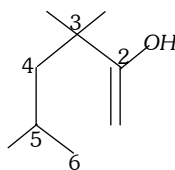


4-Hydroxy-4-methyl pentan-2-one

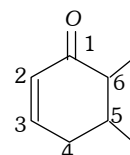
## Purification, classification and nomenclature of organic compound Part 2



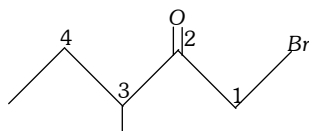
3-Ethyl penta-1, 3-diene



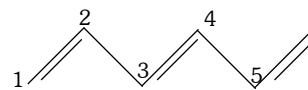
3, 3, 5-trimethylhex-1-en-2-ol



5, 6-Dimethylcyclohex-2-en-1-one



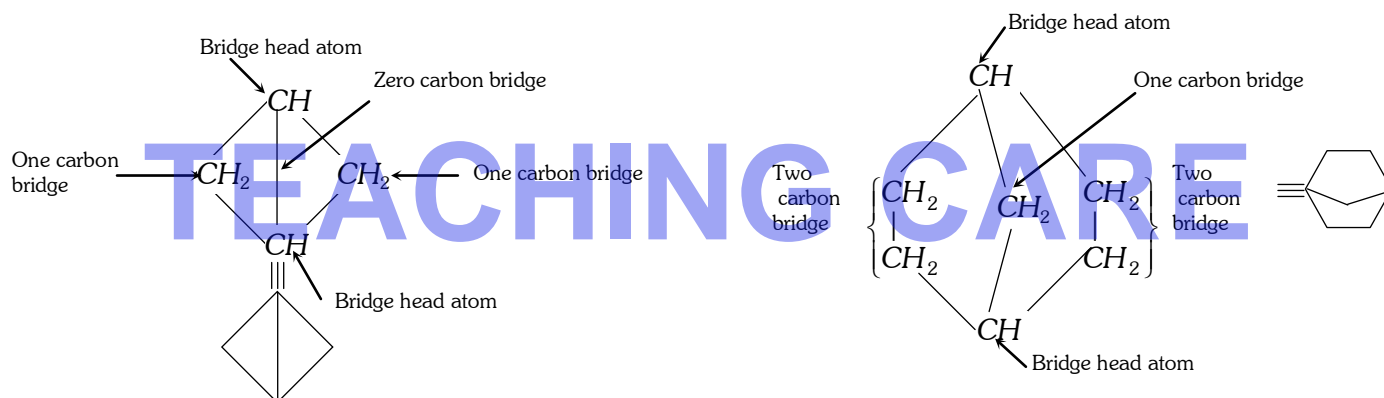
1-Bromo-3-methyl pentan-2-one



Hexa-1, 3, 5-triene

### Nomenclature of Bicyclic compounds

Many hydrocarbons and their derivatives contain two fused or bridged rings. The carbon atoms common to both rings are called bridge head atoms and each bond or chain of carbon atoms connecting both the bridge head atoms is called as bridge. The bridge may contain 0, 1, 2.... etc. carbon atoms. For example,



These bicyclic compounds are named by attaching the prefix '*bicyclo*' to the name of the hydrocarbon having the same total number of carbon atoms as in the two rings. The number of carbon atoms in each of the three bridges connecting the two bridge head carbon atoms is indicated by arabic numerals, *i.e.*, 0, 1, 2....etc. These arabic numerals are arranged in descending order; separated from one another by full stops and then enclosed in square brackets. The complete IUPAC name of the hydrocarbon is then obtained by placing these square brackets containing the arabic numerals between the prefix bicyclo and the name of alkane. For example,



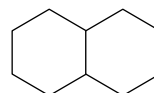
Bicyclo [2, 2, 1] heptane  
(also called norbornane)



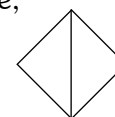
Bicyclo [3, 1, 1] heptane



Bicyclo [2, 2, 2] octane

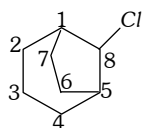


Bicyclo [4, 4, 0] decane  
(also called decalin)

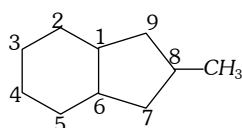


Bicyclo [1, 1, 0] butane

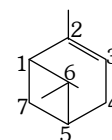
If a substituent is present, the bicyclic ring system is numbered. The numbering begins with one of the bridge head atoms, proceeds first along the longest bridge to the second bridge head atom, continues along the next longest bridge to the first bridge head atom and is finally completed along the shortest path. For example,



8-Chlorobicyclo [3, 2, 1] octane



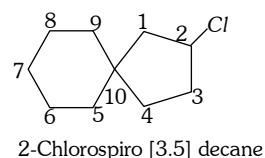
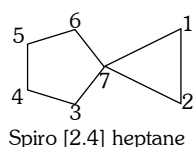
8-Methylbicyclo [4, 3, 0] nonane



2, 6, 6-Trimethylbicyclo [3, 1, 1] hept-2-ene

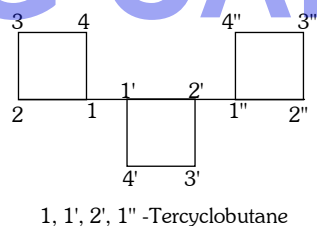
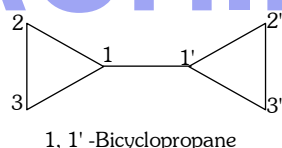
## Nomenclature of spiro compounds

Compounds in which one carbon atom is common to two different rings are called **spiro compounds**. The IUPAC name for a spiro compound begins with the word spiro followed by square brackets containing the number of carbon atoms, in ascending order, in each ring connected to the common carbon atom and then by the name of the parent hydrocarbon corresponding to the total number of the carbon atoms in the two rings. The position of substituents are indicated by numbers; the numbering beginning with the carbon atom adjacent to the common carbon and proceeding first around the smaller ring and then around the larger ring and finally ending on the common carbon atom. For example,

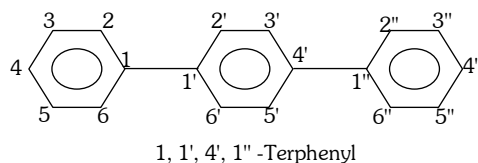


## Nomenclature of special compounds

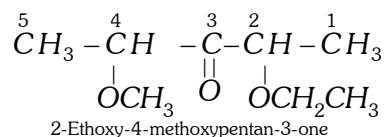
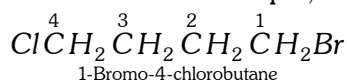
Unbranched assemblies consisting of two or more identical hydrocarbon units joined by a single bond are named by placing a suitable numerical prefix such as *bi* for two, *ter* for three, *quater* for four, *quinque* for five etc. before the name of the repetitive hydrocarbon unit. Starting from either end, the carbon atoms of each repetitive hydrocarbon unit are numbered with unprimed and primed arabic numerals such as 1, 2, 3, ..., 1', 2', 3', ..., 1'', 2'', 3'', ... etc. The points of attachment of the repetitive hydrocarbon units are indicated by placing the appropriate locants before the name. For example,



As an exception, unbranched assemblies consisting of benzene rings are named by using appropriate prefix with the name phenyl instead of benzene. For example,

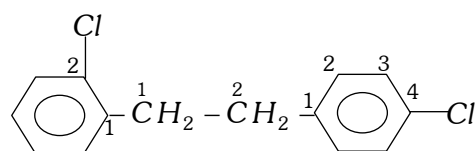


**Note** : \*If two atoms/groups of same preference occupy identical positions from either end of the parent chain, the lower number must be given to the atom/group whose prefix comes first in the alphabetical order. For example,



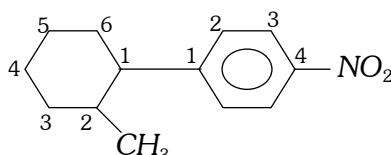
\*When two or more prefixes consist of identical words, the priority for citation is given to that group which contains the lowest locant at the first point of difference. For example,

## Purification, classification and nomenclature of organic compound Part 2



1-(2-chlorophenyl)-2-(4-chlorophenyl) ethane

✱ If a compound contains a benzene ring coupled to an alicyclic ring, it is named as a derivative of benzene, i.e. compound having lowest state of hydrogenation. For example,



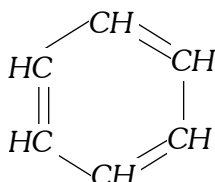
1-(2-Methylcyclohexyl)-4-nitro benzene

✱ In the common system of nomenclature, prefixes iso and neo are used only for compounds containing an isopropyl group,  $(CH_3)_2CH$  and a tert-butyl group,  $(CH_3)_3C$  respectively at the end of the carbon chain.

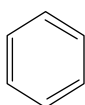
### Nomenclature of simple aromatic compounds

Aromatic compounds are those which contain one or more benzene rings in them. An aromatic compound has two main parts : (1) Nucleus, (2) Side chain

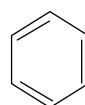
(1) **Nucleus** : The benzene ring represented by regular hexagon of six carbon atoms with three double bonds in the alternate positions is referred to as **nucleus**. The ring may be represented by any of the following ways,



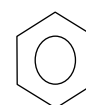
(i)



(ii)

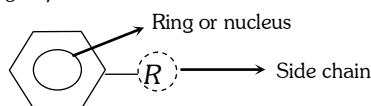


(iii)



(iv)

(2) **Side chain** : The alkyl or any other aliphatic group containing at least one carbon atom attached to the nucleus is called **side chain**. These are formed by replacing one or more hydrogen atoms in the ring by alkyl radicals i.e., R (R may be  $-CH_3$ ,  $-C_2H_5$ ,  $-C_3H_7$  etc.)



If one atom of hydrogen of benzene molecule is replaced by another atom or group of atoms, the derivative formed is called **monovalent substituted derivative**. It can exist only in one form because all the six hydrogens of benzene represent equivalent positions. For example,  $C_6H_5X$ , where X is a monovalent group.

When two hydrogen atoms of benzene are replaced by two monovalent atoms or group of atoms, the resulting product can have three different forms. These forms are distinguished by giving the numbers. The position occupied by one of the substituent is given as 1 and the other position is numbered in a clockwise direction.

(i) **Ortho** (or 1, 2-) : The compound is said to be ortho (or 1, 2-) if the two substituents are on the adjacent carbon atoms.

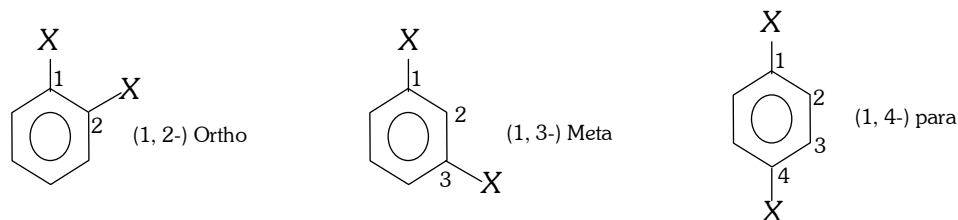
(ii) **Meta** (or 1, 3-) : The compound is said to be meta or (1, 3-) if the two substituents are on alternate carbon atoms.



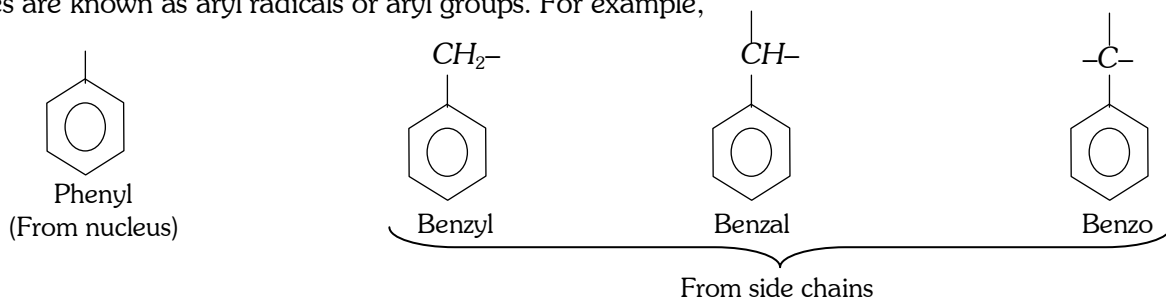
## Purification, classification and nomenclature of organic compound Part 2

(iii) **Para** (or 1, 4-) : The compound is said to be para or (1, 4-) if the two substituents are on diagonally situated carbon atoms.

Ortho, meta and para are generally represented as *o*-, *m*- and *p*- respectively as shown below,

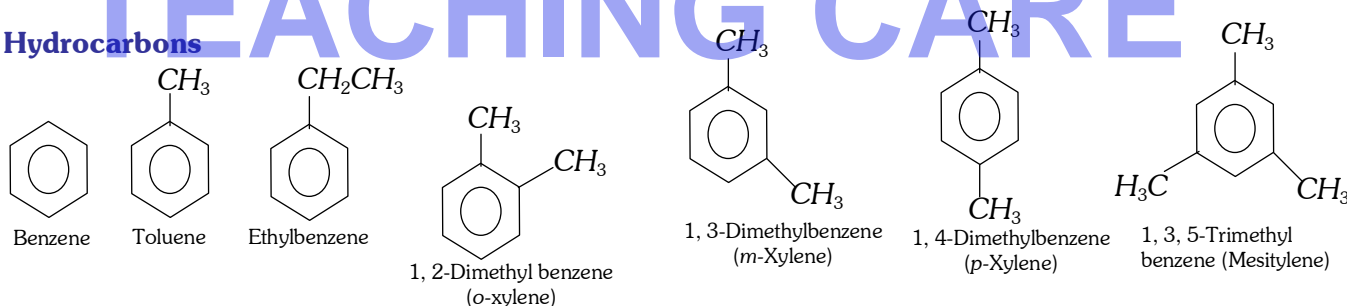


**Aryl group** : The radicals obtained by removal of one or more hydrogen atoms of the aromatic hydrocarbon molecules are known as aryl radicals or aryl groups. For example,

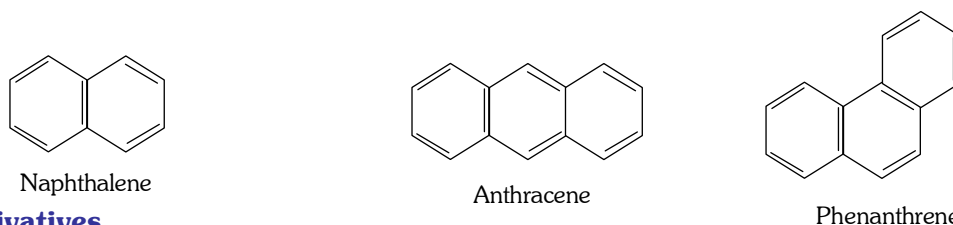


**Nomenclature of different aromatic compounds** : The names of few simple aromatic compounds are given below :

### Hydrocarbons

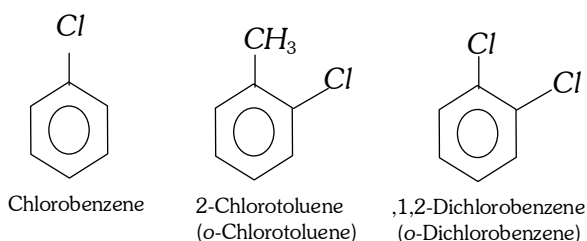


The aromatic hydrocarbons may also contain two or more benzene rings condensed together.

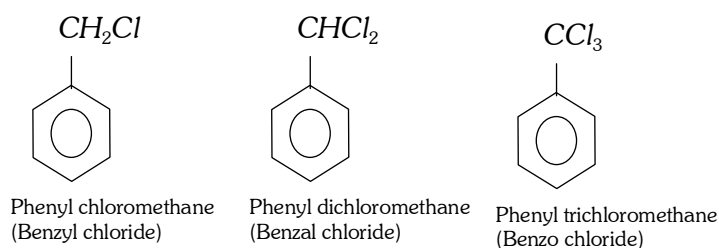


### Halogen derivatives

#### Nuclear substituted



#### Side chain substituted

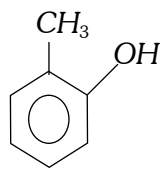


## Purification, classification and nomenclature of organic compound Part 2

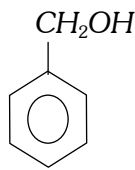
### Hydroxy derivatives



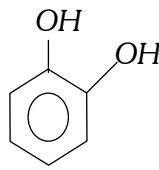
Phenol



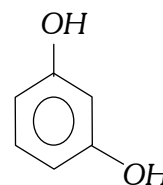
2-Methyl phenol  
o-Cresol



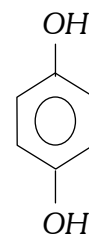
Benzyl alcohol



1, 2-Dihydroxybenzene  
(Catechol)

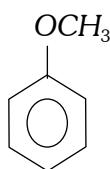


1, 3-Dihydroxybenzene  
(Resorcinol)

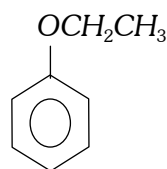


1, 4-dihydroxybenzene

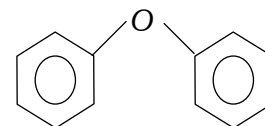
### Ethers



Methoxybenzene  
(Anisole)

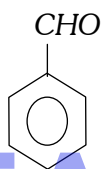


Ethoxybenzene

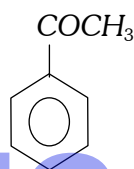


Phenoxybenzene  
(Phenetole)

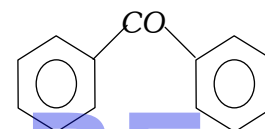
### Aldehydes and ketones (Nuclear substituted)



Benzaldehyde

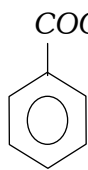


Methyl phenyl ketone  
(Acetophenone)

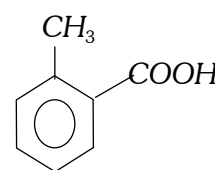


Diphenyl ketone  
(Benzophenone)

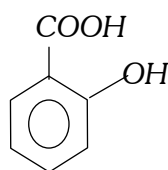
### Carboxylic acids (Nuclear substituted)



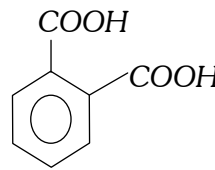
Benzoic acid



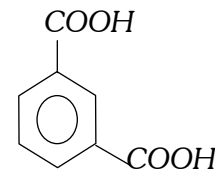
o-Toluic acid



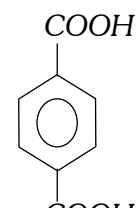
2-Hydroxy benzoic acid  
(o-salicylic acid)



Phthalic acid

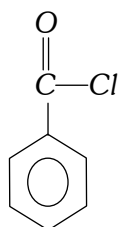


Isophthalic acid

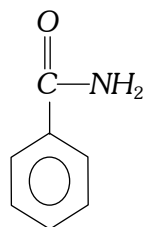


Terephthalic acid

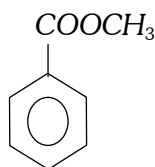
### Acid derivatives



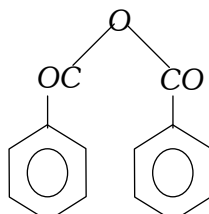
Benzoyl chloride



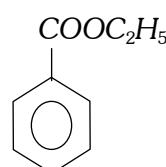
Benzamide



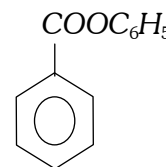
Methyl benzoate



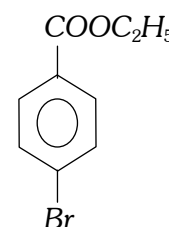
Benzoic anhydride



Ethyl benzoate



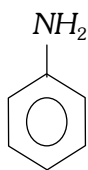
Phenyl benzoate



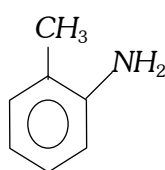
Ethyl 4-bromobenzoate

## Purification, classification and nomenclature of organic compound Part 2

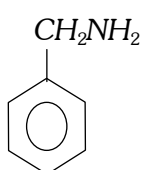
### Amino derivatives (Nuclear substituted)



Aniline (Aminobenzene)

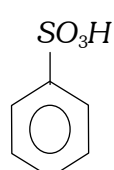


2-Amino toluene  
or  
o-Toluidine



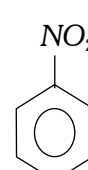
Benzyl amine

### Sulphonic acids

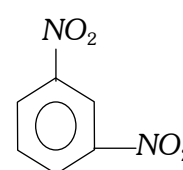


Benzene sulphonic acid

### Nitro derivatives



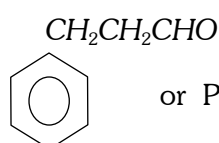
Nitrobenzene



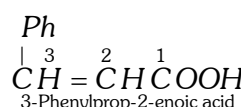
1, 3-Dinitrobenzene  
(*m*-Dinitrobenzene)

**Some tips for nomenclature of aromatic compounds :** For IUPAC nomenclature of substituted benzene compounds, the substituent is placed as prefix to the word benzene. It may be noted that common names of many substituted benzene compounds are still universally used. Some important tips for nomenclature of organic compounds are given below,

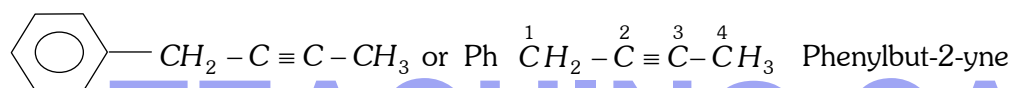
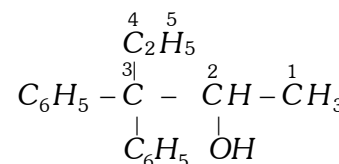
(i) When the benzene ring is named as substituent on the other molecule, it is named as **phenyl group**. It is treated in the nomenclature just like the name of an alkyl group. It is abbreviated as Ph. For example,



or Ph  $CH_2CH_2CHO$  3-Phenylpropanal

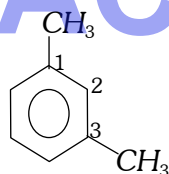


3-Phenylprop-2-enoic acid

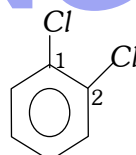


or Ph  $CH_2 - C \equiv C - CH_3$  Phenylbut-2-yne

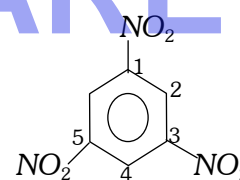
(ii) Disubstituted, trisubstituted or tetrasubstituted benzenes are named by using the numbers for the positions of the substituents.



1, 3-Dimethyl benzene



1, 2-Dichlorobenzene



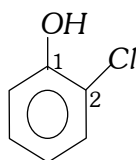
1, 3, 5-Trinitrobenzene

(iii) If different groups are attached to the benzene ring, then the following rules are *kept in mind*,

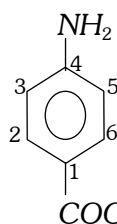
(a) The principal group is fixed as number 1.

(b) The numbering of the chain is done in any direction (clockwise or anticlockwise) which gives lower number to the substituent.

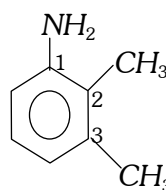
(c) The substituents are written in alphabetical order. For example,



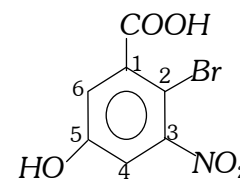
2-Chlorophenol



4-Aminobenzoic acid  
(-COOH is principal group)

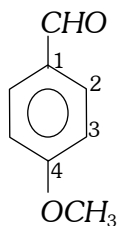


2, 3-Dimethyl aniline

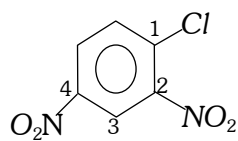


2-Bromo-5-hydroxy-  
3-nitrobenzoic acid

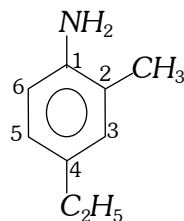
## Purification, classification and nomenclature of organic compound Part 2



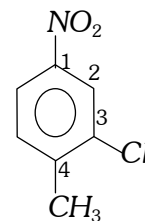
4-Methoxy benzaldehyde



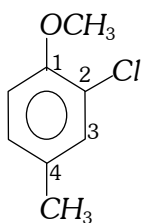
1-Chloro, 2, 4, dinitrobenzene



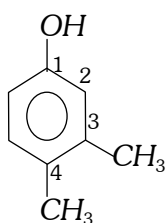
4-Ethyl-2-methylaniline



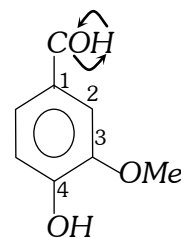
3-Chloro-4-methyl nitrobenzene



2-Chloro-4-methyl anisole



3, 4-Dimethylphenol



4-Hydroxy-3-methoxy benzaldehyde

# TEACHING CARE