

Aromatic Compounds

1 - Nomenclature

Dr. Sapna Gupta

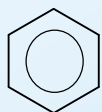
Aromatic Nomenclature

The main aromatic compound we will be covering is benzene, hence that is also the nomenclature we will focus on.

Benzene can be drawn with the alternate double bonds or with a circle inside as it has resonance of the pi bonds delocalized all over the ring. When there is a substitution on the ring, benzene is called phenyl. When there is a CH_2 group attached to the benzene, that whole group is called benzyl. (*It is easy to confuse phenyl with benzyl*).

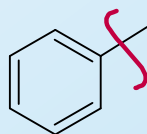
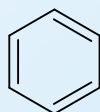
Arene (Ar-H) is the generic term for an aromatic hydrocarbon

- The aryl group (Ar) is derived by removal of a hydrogen atom from an arene



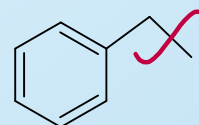
Benzene, C_6H_6

Arene



Phenyl (Ph), C_6H_5-

Aryl

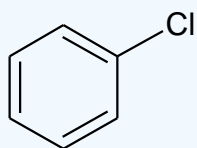


Benzyl, $\text{C}_6\text{H}_5\text{CH}_2-$

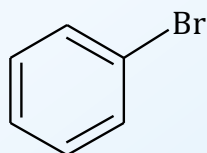
$\text{PhCH}_2\sim$

Nomenclature of Benzene - Monosubstitution

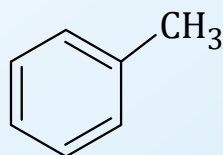
In the monosubstitution of benzene, there can be two names: the IUPAC and the general. In all the examples here, I have given the IUPAC name first.



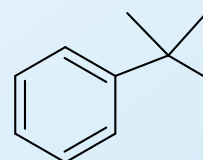
Chlorobenzene
Phenylchloride



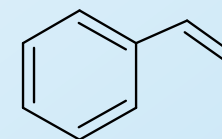
Bromobenzene
Phenylbromide



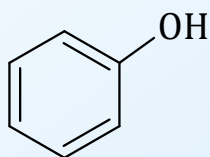
Methylbenzene
Toluene



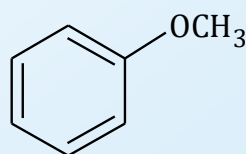
T-butylbenzene
Toluene



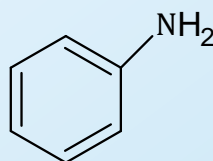
Vinylbenzene
Styrene



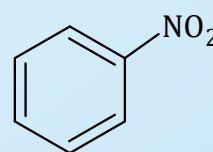
Phenol
Hydroxybenzene
Phenylalcohol



Methoxybenzene
Anisole
Methyl phenyl ether



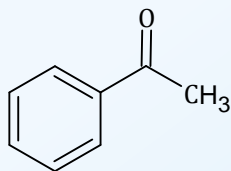
Aniline
Aminobenzene



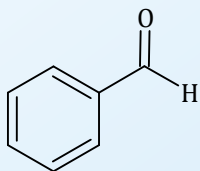
Nitrobenzene

Nomenclature of Benzene Contd...

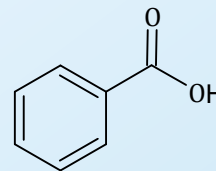
In the structures that have a carbonyl group on benzene, there is complete change in the name and in some cases, there is only one name.



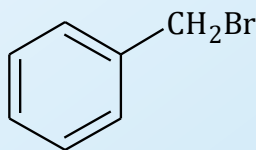
Acetophenone



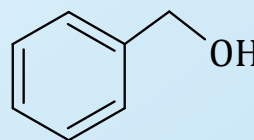
Benzaldehyde



Benzoic acid



Benzylbromide



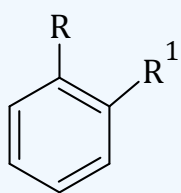
Benzyl alcohol
PhCH₂OH

Phenyl and Benzyl

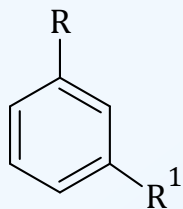
Phenyl indicates the benzene ring attachment. The benzyl group has an additional carbon.

Disubstituted Benzene Derivatives

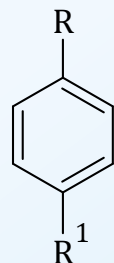
The prefixes *ortho*-, *meta*-, and *para*- are commonly used for the 1,2-, 1,3- and 1,4-positions, respectively.



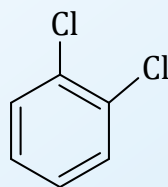
1,2-
ortho



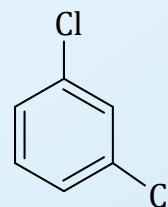
1,3-
meta



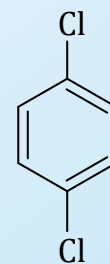
1,4-
para



1,2-dichlorobenzene
o-dichlorobenzene

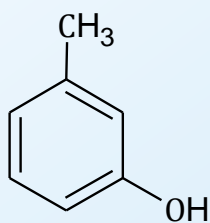


1,3-dichlorobenzene
m-dichlorobenzene

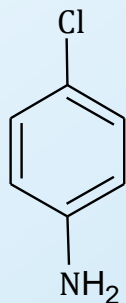


1,4-dichlorobenzene
p-dichlorobenzene

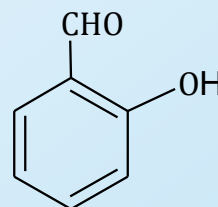
Some more di substituted compounds with common names.



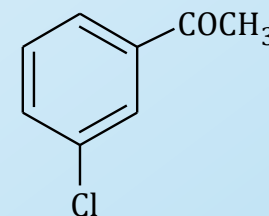
M-hydroxytoluene
M-methylphenol
3-methylhydroxybenzene



p-chloroaniline
4-chloroaminobenzene



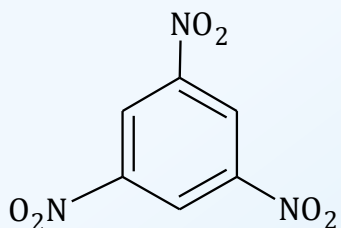
O-hydroxybenzaldehyde



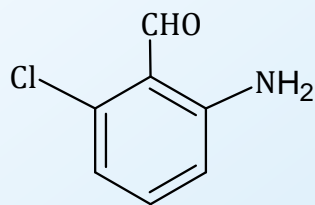
M-chloroacetophenone

Trisubstituted Benzene Derivatives

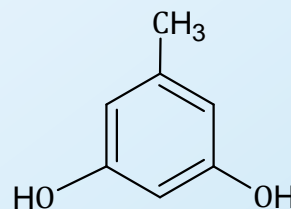
To name the trisubstituted benzenes, find the substituent that you want to give the base name of benzene to, e.g. phenol, benzaldehyde etc. That will be your 1st substituent. Now number all other substituents giving them low numbers and name them in alphabetical order.



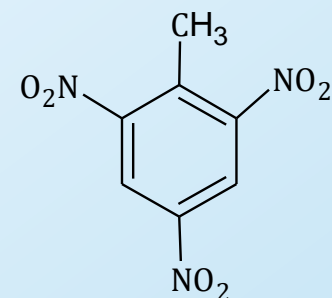
1,3,5-trinitrobenzene



2-amino-6-chlorobenzaldehyde

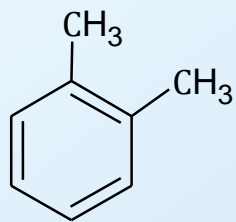


3,5-dihydroxytoluene

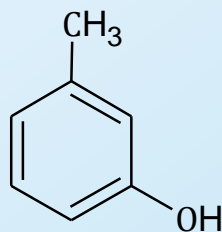


2,4,6-trinitrotoluene (TNT)

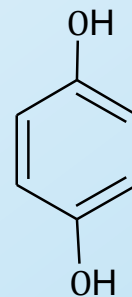
Some common names of diols and alkyl benzenes.



O-xylene



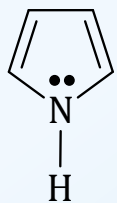
M-cresol



hydroquinone

Heterocyclic Aromatics

Heterocyclic aromatics have at least one atom other than carbon in the ring. Nitrogen, oxygen and sulfur are common atoms that occur in ring structures. Their names are unique and usually the general names are used.



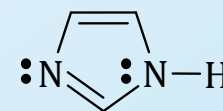
Pyrrole



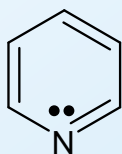
Furan



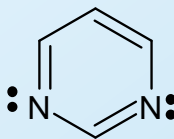
Thiophene



Imidazole



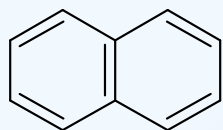
Pyridine



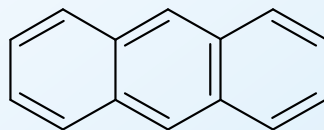
Pyrimidine

Polynuclear Aromatics

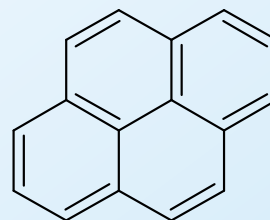
Benzene rings fused together are called polynuclear rings. These are inherently aromatic compounds. There can be 2, 3 or more rings fused together.



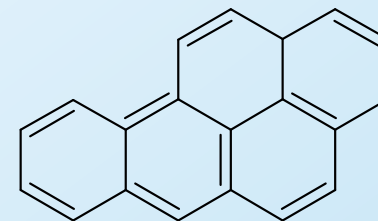
Naphthalene



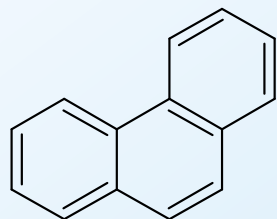
Anthracene



Pyrene

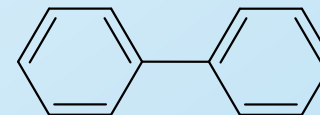


Benzo[a]pyrene



Phenanthrene

Benzene rings joined together with a bond is called biphenyl.



Physical Properties

- 1) Boiling Points: Benzene compounds higher boiling points than alkanes because of high molecular weight.
- 2) Solubility: Benzene and derivatives are not soluble in water due to non polar nature of the ring.
- 3) Density: It can be lower or greater than water depending on the substituents. Benzene and small alkylbenzenes are lighter than water.
- 4) Odor: Aromatic compounds have an odor hence the name aromatics.

Applications of Aromatics

- Solvents – Due to its lack of reactivity, benzene and alkyl benzenes are good solvents for organic reactions.
- Pharmaceuticals – A number of medications have benzene rings as their base structure (aspirin, acetaminophen, ibuprofen etc) or as substituent groups to create a nonpolar group.
- Naphthalene – is the common moth balls used as a disinfectant.
- Styrene – is the compound used as a monomer to make polystyrene, one of the most common polymer.
- Benzoic acid – is used as a preservative.
- Benzopyrenes – are formed in the byproduct of tobacco and is a potent carcinogen.

Needless to say benzene and its derivatives are highly interwoven in our lives.

Key Concepts

- IUPAC and general names of benzene and its mono substituted derivatives.
- Nomenclature of di and tri substituted benzene.