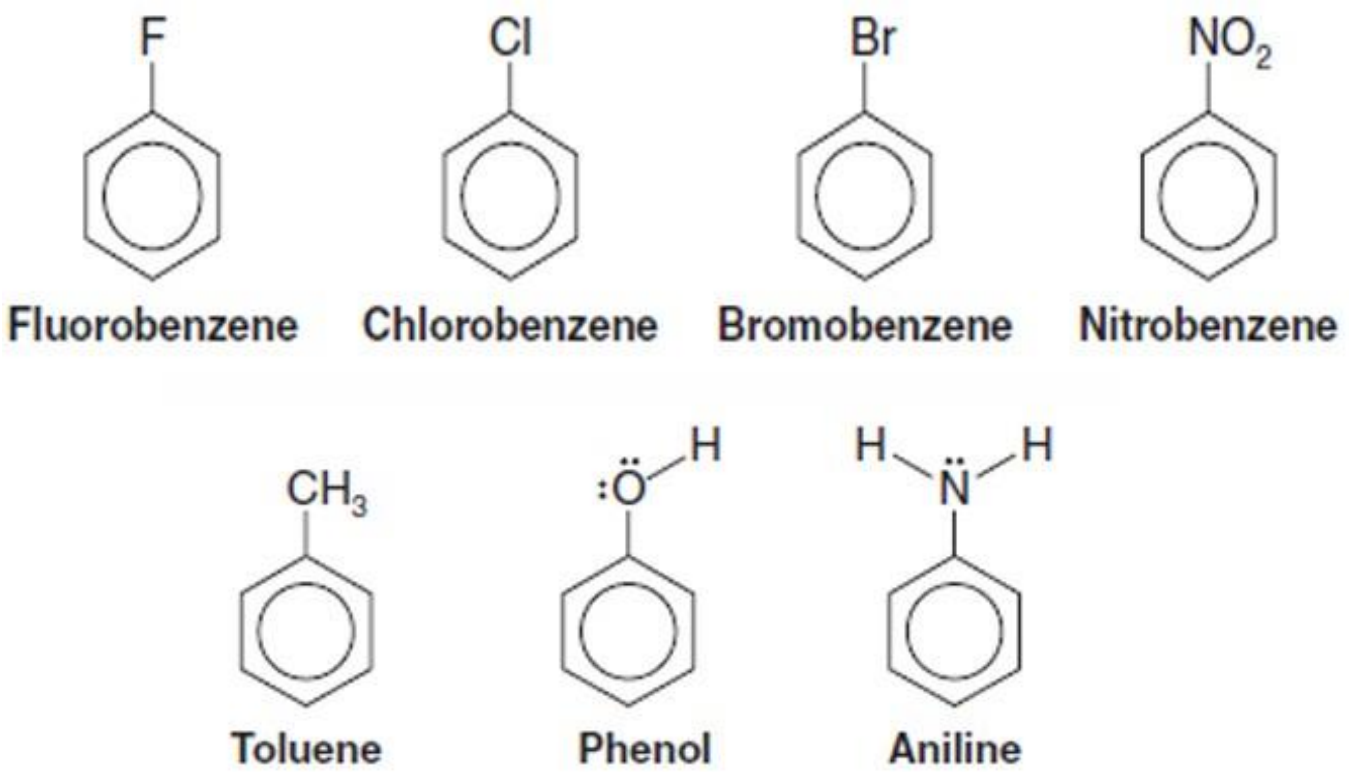
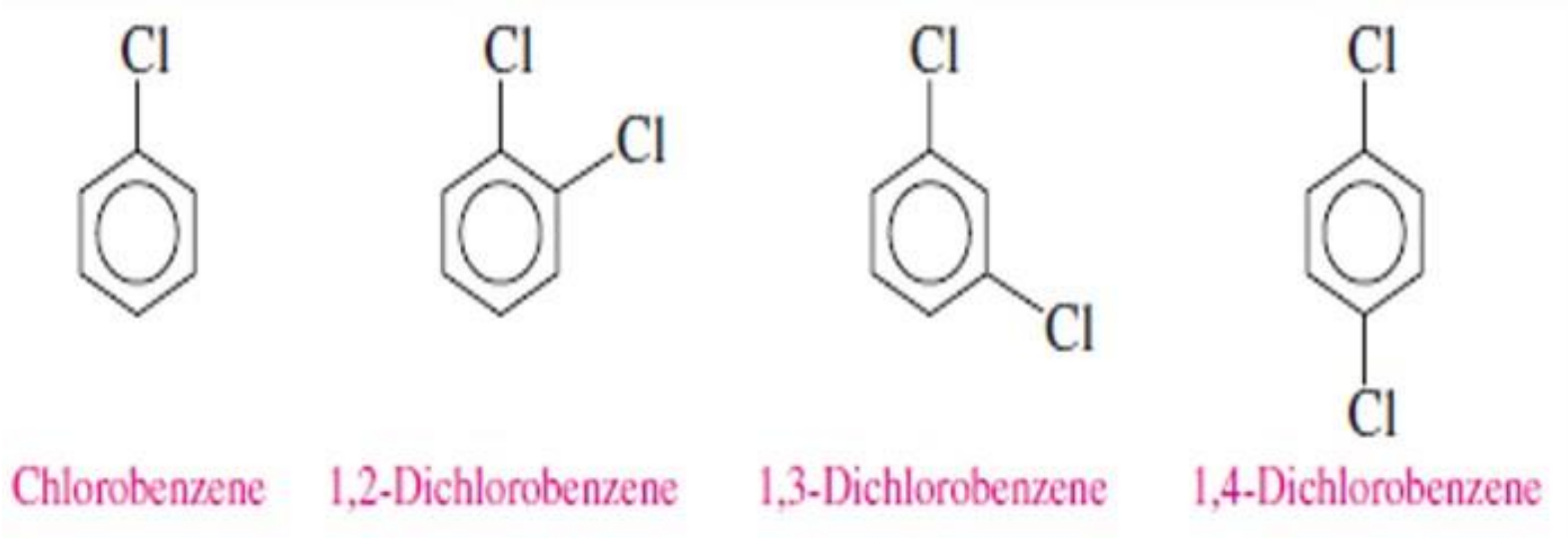
Nomenclature of Benzene Derivatives

➢ Monosubstituted:

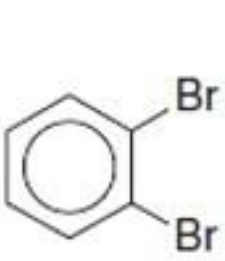
Two systems are used in naming Monosubstituted benzenes. In many simple compounds, benzene is the parent name and the substituent is simply indicated by a prefix. For example:



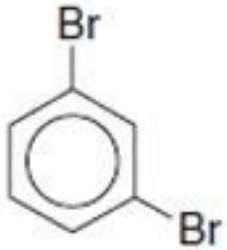
When benzene has only one substituent, the benzene ring is not numbered. When there are two or more substituents, the benzene ring is numbered to give the lower numbers to the substituents.



When two substituents are present, their relative positions are indicated by the prefixes ortho-, meta-, and para- (abbreviated o-, m-, and p-) or by the use of numbers.

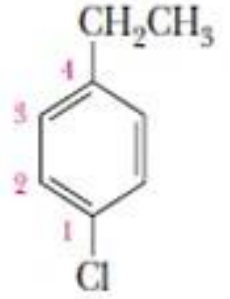


1,2-Dibromobenzene
(*o*-dibromobenzene)
ortho



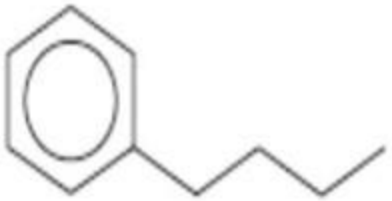
1,3-Dibromobenzene
(*m*-dibromobenzene)
meta

1,4-Dibromobenzene
(*p*-dibromobenzene)
para

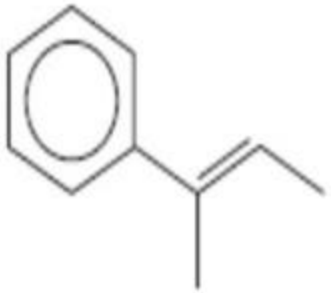


1-Chloro-4-ethylbenzene
(*p*-Chloroethylbenzene)

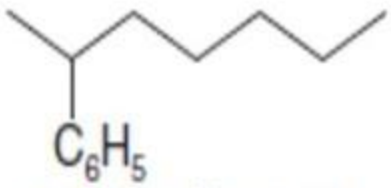
When the C_6H_5- group is named as a substituent, it is called a phenyl group. The phenyl group is often abbreviated as C_6H_5- or Ph- When a hydrocarbon composed of one saturated chain and one benzene ring is usually named as a derivative of the larger structural unit. However, if the chain is unsaturated, the compound may be named as a derivative of that chain, regardless of ring size. The following are examples



Butylbenzene

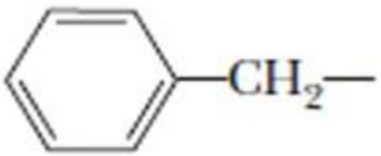


2-Phenyl-2-butene

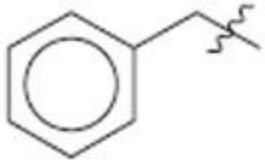


2-Phenylheptane

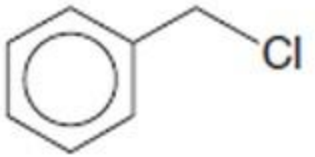
Benzyl is an alternative name for the phenylmethyl group. It is sometimes abbreviated Bn.



Benzyl group, Bn–



The benzyl group (the phenylmethyl group)



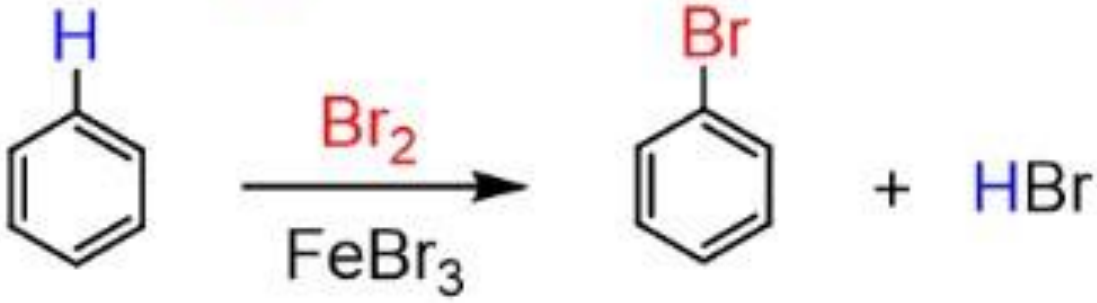
Benzyl chloride (phenylmethyl chloride or BnCl)

Electrophilic Aromatic Substitution – The Mechanism

Benzene has 3 π bonds and as expected shows some similarities to alkenes in being reactive towards electrophilic species. However, there are two key differences between their reactions with electrophiles.

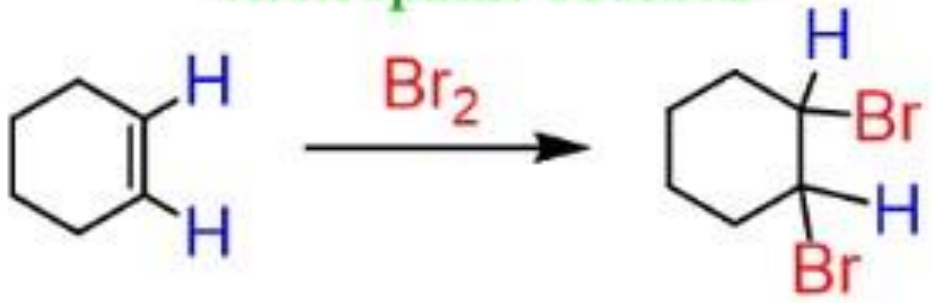
First, benzene is very stable and thus less reactive. Second, unlike the alkenes, it undergoes an electrophilic substitution and not an electrophilic addition reaction:

electrophilic substitution



The H has been replaced by the Br

electrophilic addition



Two Br have been added to the double bond

The first difference of benzene being less reactive brings the need for using a Lewis acid $FeBr_3$ which turns the Br_2 into a stronger electrophile and makes the reaction possible. We will see how that works next.

The second difference is that the Br in the electrophilic aromatic substitution reaction replaces the hydrogen while both hydrogens are still there when they are on the alkene. And in fact, this is still related to the **stability of the aromatic ring**. Even though the reaction goes through an intermediate where the aromaticity is broken, it still ends up restored because that brings a lot of stability and energetically is very favorable.

Reaction of Benzene