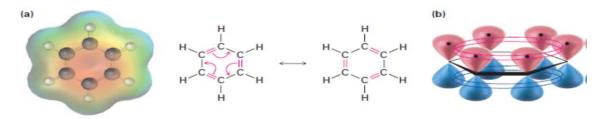
Aromatic Compounds

A large class of unsaturated <u>chemical compounds</u> characterized by one or more planar rings of <u>atoms</u> joined by <u>covalent bonds</u>. have a special properties, including unusual stability, due to their aromaticity. They are often represented as resonance structures containing single and double bonds.

Structure of Aromatic Compounds

Aromatic compounds are cyclic structures in which each ring atom is a participant in a sigma δ and pi π bond, resulting in delocalized sigma δ and pi π electron density on both sides of the ring. Due to this connected network of sigma δ and pi π bonds, the rings are planar, unlike the boat or table structures typical of cycloalkanes.



Benzene can only be fully depicted with all of its resonance structures, which show how its pi-electrons are delocalized throughout its six-carbon ring. This delocalization leads to a lower overall energy for the molecule, giving it greater stability.

Physical Properties of Aromatic Compounds

- 1-Aromatic compounds are generally nonpolar and immiscible with water.
- 2-As they are often unreactive, they are useful as solvents for other nonpolar compounds.
- 3-Due to their high ratio of carbon to hydrogen, aromatic compounds are characterized by a sooty yellow flame

Sources of Aromatic Hydrocarbons

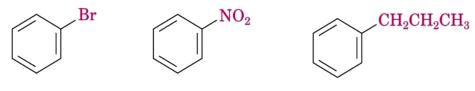
- From high temperature distillation of coal tar
- Heating petroleum at high temperature and pressure over a catalyst

Naming Aromatic Compounds

Many common names (toluene = methylbenzene; aniline = amino benzene)

Mono substituted benzenes systematic names as hydrocarbons with – benzene

- $C_6H_5Br =$ bromo benzene
- $C_6H_5NO_2 =$ nitrobenzene, and
- C₆H₅CH₂CH₂CH₃ is propyl benzene

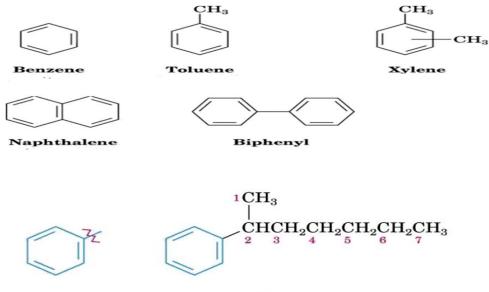


Bromobenzene

Nitrobenzene

Propylbenzene

The Phenyl Group When a benzene ring is a substituent, the term phenyl is used (for C_6H_5)

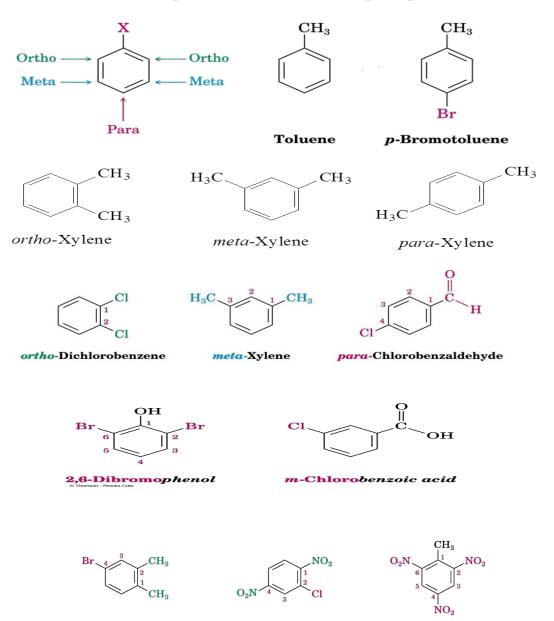


A phenyl group

2-Phenylheptane

Di substituted Benzenes

- Relative positions on a benzene ring
 - *ortho- (o)* on adjacent carbons (1,2)
 - *meta-* (*m*) separated by one carbon (1,3)
 - *para-* (*p*) separated by two carbons (1,4)
- Describes reaction patterns ("occurs at the para position")



4-Bromo-1,2-dimethylbenzene

2-Chloro-1,4-dinitrobenzene

2,4,6-Trinitrotoluene (TNT)

Benzene (C₆H₆)

Is the best-known aromatic compound. The six carbons of benzene are joined in a ring, having the planar geometry of a regular hexagon in which all of the C—C bond distances are equal. The six π electrons circulate in a region above and below the plane of the ring, each electron being shared by all six carbons, which maximizes the force of attraction between the nuclei (positive) and the electrons (negative).

1-Benzene has two resonance forms

2-The six carbon - carbon bonds are of equal length, intermediate between a

single bond and double bond

3-The molecule is planar

4-The bond angle around each carbon is approximately 120°

1- The apparent hybridization orbital consistent with the geometry would

be sp^2 (trigonal planar arrangement) This would leave a single p orbital associated with each carbon (perpendicular to the plane of the ring)

Because we cannot say that the electrons in the π bonds

are localized to a particular atom they are described as being *delocalized* among the six carbon atoms.

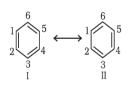
Nucleophiles and Electrophiles

A reagent that brings an electron pair is called a **nucleophile** (Nu:) i.e., nucleus seeking and the reaction is then called **nucleophilic**.

A reagent that takes away an electron pair is called **electrophile** (E+) i.e., electron seeking and the reaction is called **electrophilic**.

Benzene Reaction

As a consequence of the π electrons above and below the plane of its ring, benzene is a nucleophile. It will, therefore, react with an electrophile (Y⁺) when an electrophile attaches itself to a benzene ring, a carbocation intermediate is formed



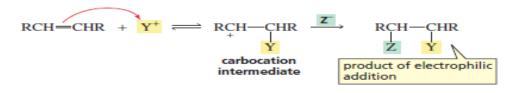




This should remind you of the:-

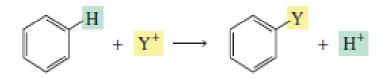
First step in an electrophilic addition reaction of an alkene: A nucleophilic alkene reacts with an electrophile, thereby forming a carbocation intermediate .

Second step of an electrophilic addition reaction, the carbocation reacts with a nucleophile (Z^{-}) to form an addition product.

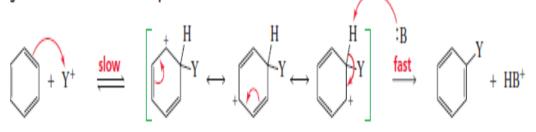


General Mechanism for Electrophilic Aromatic Substitution Reactions

In the substitution reaction, an electrophile substitutes for one of the hydrogen's attached to the benzene ring.

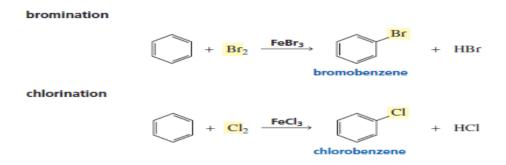


general mechanism for electrophilic aromatic substitution

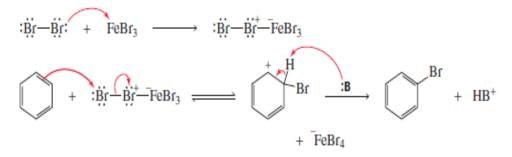


1-Halogenation of Benzene

The bromination or chlorination of benzene requires a Lewis acid such as ferric bromide or ferric chloride. Recall that a *Lewis acid* is a compound that accepts a share in a pair of electrons.

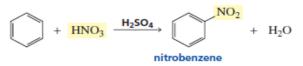


mechanism for bromination



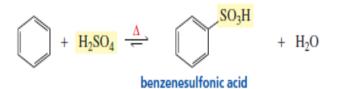
2-Nitration of Benzene

Nitration of benzene with nitric acid requires sulfuric acid as a catalyst.



3-Sulfonation of Benzene

Fuming sulfuric acid (a solution of SO_3 in sulfuric acid) or concentrated sulfuric acid is used to sulfonate aromatic rings.

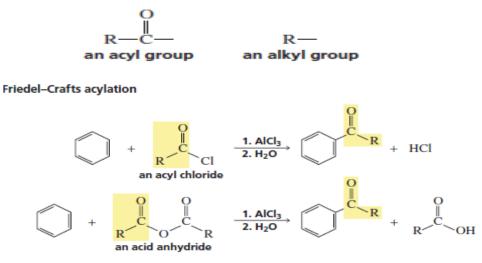


4-Friedel–Crafts Acylation of Benzene

Two electrophilic substitution reactions bear the names of chemists Charles Friedel and James Crafts.

(Friedel-Crafts acylation)places an acyl group on a benzene ring.

Friedel–Crafts alkylation places an alkyl group on a benzene ring.



4-Friedel–Crafts Acylation of Benzene

The Friedel–Crafts alkylation reaction substitutes an alkyl group for a hydrogen.

