Tishk International University
Faculty of Pharmacy / 2nd Year
Practical Organic Chemistry II
Experiment 02

Preparation of Nitrobenzene

(Nitration of benzene)

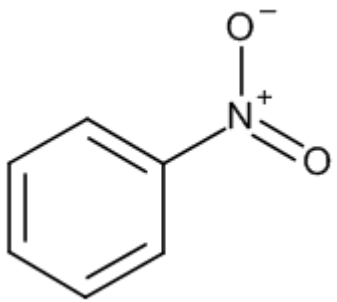
Example on
(electrophilic aromatic substitution)

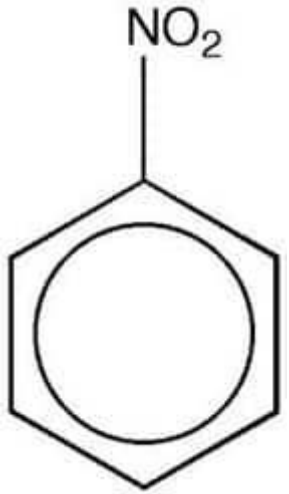
Nitrobenzene

- **Nitrobenzene**, the simplest aromatic nitro compound, having the molecular formula $\mathbf{C_6H_5NO_2}$.
- It is used in the manufacture of aniline, benzidine, and other organic chemicals.
- Nitrobenzene is a colorless to pale yellow, oily, highly toxic liquid with the odor of bitter almonds.
- Nitrobenzene was first prepared in 1834 by the German chemist Eilhardt Mitscherlich.
- Other names: **Nitrobenzol** and **Oil of mirbane**

Physical properties of nitrobenzene

Molecular Formula: $\mathbf{C_6H_5NO_2}$
Molecular Weight: 123.1094 g/mol
IUPAC Name: Nitrobenzene
Melting Point: 5.7 °C
Boiling Point: 210.9 °C
Density: 1.2 g/cm³



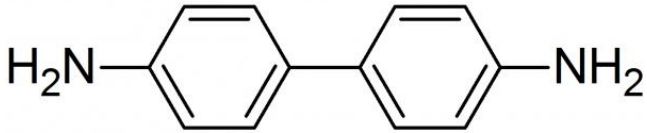


Solubility:

1. very slight to insoluble in water
2. Slightly soluble in carbon tetrachloride
3. Soluble in ethanol and acetone
4. Completely Miscible with diethyl ether and benzene

Uses of nitrobenzene

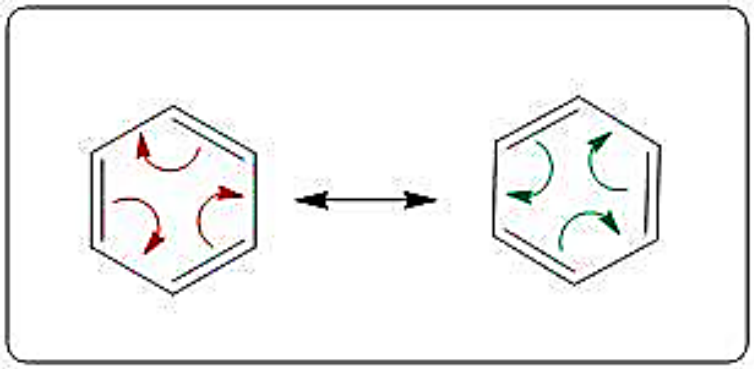
1. Approximately 95% of nitrobenzene used to produce aniline.
2. Production of acetaminophen (paracetamol).
3. Perfume for soaps due to its low cost.
4. Production of benzidine.



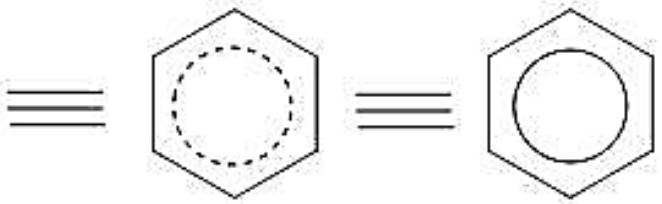
5. Nitrobenzene is also used to produce lubricating oils and in the manufacture of dyes, drugs, pesticides, and synthetic rubber

Electrophilic Aromatic Substitution (EAS)

Although aromatic compounds have multiple double bonds, these compounds do not undergo addition reactions. Their lack of reactivity toward addition reactions is due to the great stability of the ring systems that result from complete π electron delocalization (resonance).



Benzene 2 Resonance forms

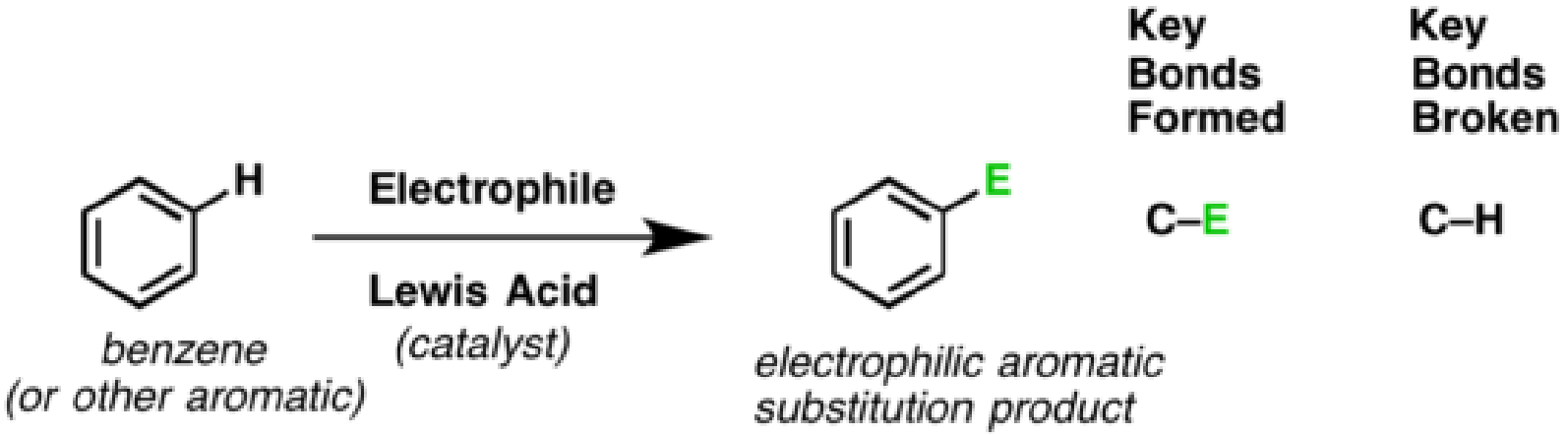


Hybrid Forms

Experiment 02
Nitration of benzene

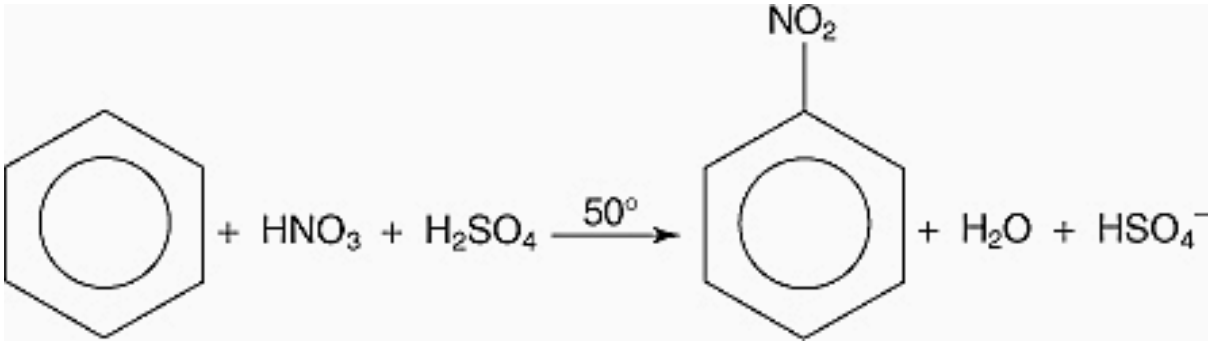
Aromatic compounds react by electrophilic aromatic substitution reactions, in which the aromaticity of the ring system is preserved.

A key reaction of aromatic compounds is electrophilic aromatic substitution, where a **C-H** bond is broken and a new **C-E** bond (**E being an electrophilic atom such as Cl, Br, N…**) is formed.



Preparation of nitrobenzene

Benzene is treated with a mixture of concentrated nitric acid and concentrated sulphuric acid at a temperature not exceeding 50°C. As temperature increases there is a greater chance of getting more than one nitro group, $-NO_2$, substituted onto the ring.



Sulfuric acid acts as a catalyst

Procedure

1. 7 ml of conc. HNO_3 is added to a round bottom flask, add 8 ml of conc. H_2SO_4 with continuous stirring, this process must be done in a ice bath.
2. Add 6 ml of benzene drop wise to the mixture, below 50 ^oC in all times.
3. After all benzene added, the solution is pale to yellow color and heated to near 55-60 ^oC (the temperature must not reach more than 60 ^oC) with continuous stirring for nearly one hour.
4. After one hour, the solution left to cool and the two immiscible layers are simply distinguished.
5. Separation funnel is used to separate the two immiscible layers from each other.
6. The lower layer is acids and the upper layer is the nitrobenzene. Which can be purified and yield percent can be found.