Xylenes and derivatives

Thitiphan Chimsook

Xylene

- A mixture of three aromatic hydrocarbon isomers
- A solvent in the printing, rubber, and leather industries
- Clear, colorless, sweet-smelling liquid
- Flammable
- Refined from crude oil in a dealkylation

Production

- Reformate from refinery
- Pyrolysis gasoline from steam cracking
- Disproportionation of toluene

Xylene is a colorless liquid, while o-xylene and p-xylene are colorless liquids and solids.
**Current use**

- Used in mixed fractions to prevent oxidation
- Used as a diluent
- Paraxylene is used to produce terephthalic acid (terephthalic acid) and coca cola in the form of ethylene glycol. It is used in the production of polyester and polyethylene terephthalate (PET)
- Orthoxylene is used to produce phthalic anhydride to be used as a plasticizer
- Paraxylene is used to produce isophthalic acid which is a precursor for the production of plasticizer

**p-Xylene**

- To produce terephthalic acid and dimethyl Terephthalate (dimethyl terephthalate) (dimethyl terephthalate) by reacting diol
- Terephthalic acid (TPA) – white solid, insoluble, dissolves in ethanol, ether, acetic acid

![Chemical structure of terephthalic acid](image)

**Production of Terephthalic acid**

- Amoco process
- p-Xylene will be oxidized with air in the liquid phase
- At 200°C and 20 atm in acetic acid
- CO, Mn and Bromide ions used as catalyst
- Reactor uses titanium (titanium has high reactivity in the reaction)
- Impurities (p-toluic acid and p-carboxybenzaldehyde) are easy to isolate

![Chemical structure of dimethyl terephthalate](image)

Colorless crystalline, insoluble, dissolves in ether and hot methanol
Production of Dimethyl Terephthalate

- Witten process
- 2 steps of oxidation and esterification
- p-xylene and methyl p-toluate react with oxygen in air by using cobalt naphthenate as catalyst.
- p-toluic acid and methyl hydrogen terephthalate as products
- These products will react with methanol at 250-280 C and 20-25 atm.
- Final products are methyl p-toluate and dimethyl terephthalate.
Poly (ethylene terephthalate)

- **PET**
- Thermoplastic polymer resin
- Used in synthetic fibers; beverage, food and other liquid containers

![Chemical structure of PET](image)

Poly (ethylene terephthalate)

- PET consists of polymerized units of the monomer ethylene terephthalate

![Chemical structure of PET](image)

Poly (ethylene terephthalate)

- Dimethyl terephthalate (DMT) or Terephthalic acid (TPA) as substrate
- Present – TPA-
- If use DMT, it will eliminate methanol

![Chemical structure of reaction](image)

Production Poly (ethylene terephthalate)

- Reaction:
  \[
  \text{HOCH}_2\text{CH}_2\text{OH} + \text{HO}_2\text{C}\text{TPA} \rightarrow \text{HOCH}_2\text{CH}_2\text{OOC}\text{CH}_2\text{CH}_2\text{OOC}\text{CH}_2\text{CH}_2\text{OOC}\text{CH}_2\text{CH}_2\text{OOC}\ldots \text{CH}_2\text{CH}_2\text{OH}
  \]
  \[n = 1-6\]
  bis-(2-hydroxyethyl) terephthalate)
Production Poly (ethylene terephthalate)

\[
\text{O}_2\text{C} - \text{CO}_2\text{CH}_2\text{CH}_2\text{OH} + \text{OHCH}_2\text{CH}_2\text{O}_2\text{C} - \text{CO}_2 \\
\rightarrow \text{HOCH}_2\text{CH}_2\text{O}_2\text{C} - \text{CO}_2 + \text{HOCH}_2\text{CH}_2\text{OH}
\]

O-Xylene

- Phthalic anhydride
- Anhydride of phthalic acid
- Colourless solid
- Industrial chemical for the production of plasticizers for plastics.

Production

- Phthalic anhydride prepared from phthalic acid

\[
\Delta \text{C}_6\text{H}_4(\text{CH}_3)_2 + 3 \text{O}_2 \rightarrow \text{C}_6\text{H}_4(\text{CO})_2\text{O} + 3 \text{H}_2\text{O}
\]

- Catalytic oxidation of o-xylene and naphthalene

\[
\text{C}_{10}\text{H}_8 + 4.5 \text{O}_2 \rightarrow \text{C}_6\text{H}_4(\text{CO})_2\text{O} + 2 \text{H}_2\text{O} + 2\text{CO}_2
\]
Current use

- To produce plasticizers by reacting with alcohol
- To produce dyes
- To produce magnesium peroxyphthalate for detergent
- To produce phenolphthalein
- To produce cross-linking for polyester resin
- To produce alkyd resin (low M.W. polyester)

**o-Xylene**

\[
\text{C}_6\text{H}_4(\text{CH}_3)_2 + 3 \text{O}_2 \rightarrow \text{C}_6\text{H}_4(\text{CO})_2\text{O} + 3 \text{H}_2\text{O}
\]

**m-Xylene**

- **Isophthalonitrile** (ไอโซฟาทาโลไนทริล)

\[
\text{CH}_3
\]

- Produced from m-xylene with ammoxidation process
• Used as the precursor to produce the deconil (ยาฆ่าเชื้อรา) with chlorination process

\[
\begin{align*}
\text{CN} & \quad \text{4Cl}_2 \\
\text{Deconil} & \quad \text{CN} \quad \text{Cl} \quad \text{Cl} \quad \text{Cl} \quad \text{CN} \\
& + \quad 4\text{HCl}
\end{align*}
\]

• Isophthalic acid

- colourless solid

\[
\begin{align*}
\text{HO} & \quad \text{C} \quad \text{HO} \\
\text{Isophthalic acid} & \quad \text{C} \quad \text{OH}
\end{align*}
\]

- Isomer of phthalic acid and terephthalic acid.

Current use

• To produce isophthaloyl chloride

• Isophthaloyl chloride react with m-phenylene diamine to get aramid polymer (nomex, สมบัติทนร้อนสูง ทำเสื้อผ้ากันไฟไหม้ของนักดับเพลิง)