CL304 REPORT

PRODUCTION OF BTX(Benzene, Toluene & Xylene)

GROUP-8

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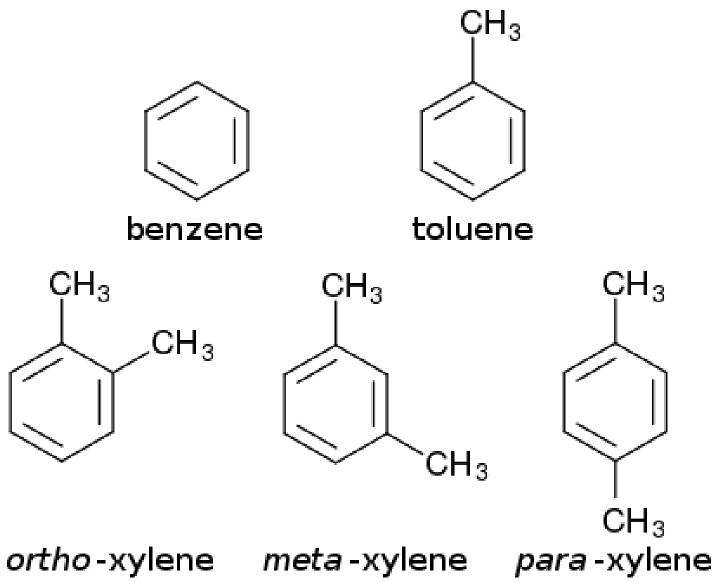
INTRODUCTION TO BTX:

The initials BTX denote mixes of aromatic hydrocarbons, namely **benzene**, **toluene**, and the **three isomers of xylene**, used in the petroleum refining and petrochemical industries.The xylene isomers are distinguished by the designations *ortho* – (or *o* –), *meta* – (or *m* –), and *para* – (or *p* –) forms. All the three components of BTX are aromatic hydrocarbons with similar structures.



PROPERTIES OF BTX HYDROCARBONS:

1)BENZENE(C6H6):

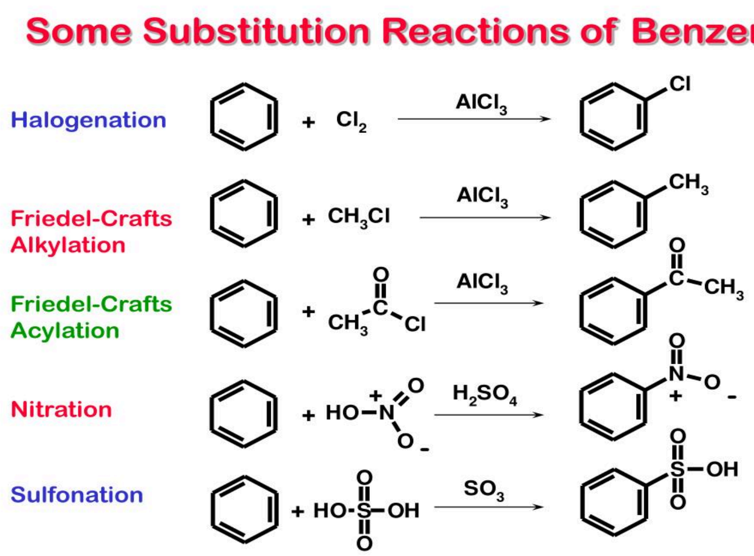
Physical Properties:

- Benzene is a colourless, volatile liquid at room temperature and pressure (25°C and 1 atm).
- It has a distinctive sweet odour, which is often described as aromatic.
- Benzene has a density of about 0.879 g/cm^3 and a melting point of 5.5°C.
- The boiling point of benzene is 80.09°C.
- It is highly flammable, with a flash point of -11°C, and forms explosive mixtures with air.

Chemical Properties:

1. Substitution Reactions:

- Due to its aromatic nature, benzene undergoes substitution reactions rather than addition reactions.
- These reactions involve the replacement of hydrogen atoms with other functional groups.
- Some common substitution reactions of Benzene include nitration (NO2 group substitution), sulfonation (sulfonic acid group substitution), halogenation (halogen atom substitution), and alkylation/acylation (alkyl or acyl group substitution).



2. Oxidation Resistance:
    - Benzene is generally resistant to oxidation under normal conditions.
    - However, under more vigorous conditions, it can be oxidized to form phenol or benzoic acid.
3. Benzene is toxic and a known carcinogen, with exposure linked to leukaemia and other health issues.

2)TOLUENE(C7H8):

Physical Properties:

- Toluene is a colourless liquid at room temperature.
- It has a sweet, pungent odour.
- Toluene has a melting point of -93°C and boiling point of 110.6°C. The density of Toluene is 0.867g/cm^3.
- Toluene is immiscible with water but soluble in organic solvents like ethanol and acetone.

- Toluene is highly flammable with a flash point of 4.4°C.It forms explosive mixtures with air within certain concentration ranges.
- It is not corrosive to most metals.

Chemical Properties:

- Toluene is relatively stable but can react under certain conditions, such as with strong oxidizing agents.
- It undergoes typical reactions of aromatic hydrocarbons such as electrophilic substitution reactions.
- Some common substitution reactions of toluene include nitration (NO_2 group substitution), sulfonation (sulfonic acid group substitution), halogenation (halogen atom substitution), and alkylation/acylation (alkyl or acyl group substitution).
- **Oxidation Resistance**:Toluene is generally resistant to oxidation under normal conditions, similar to benzene. However, under more vigorous conditions, toluene can be oxidized. It may undergo oxidation to form compounds such as benzyl alcohol, benzaldehyde, or benzoic acid, depending on the reaction conditions and oxidizing agents used.
- Toluene vapour can cause health issues like headaches, dizziness, and in high concentrations, central nervous system depression.

3)XYLENE(C_8H_{10}):

Physical Properties:

- Xylene refers to a group of three isomeric aromatic hydrocarbons: ortho-xylene, meta-xylene, and para-xylene.
- Xylene is a colourless, flammable liquid at room temperature.
- It has a characteristic sweet, aromatic odour, similar to benzene and toluene.
- The density of xylene varies depending on the isomer and temperature, but it typically ranges from about 0.86 to 0.88 g/cm^3 at room temperature.
- The melting points of the isomers are as follows: ortho-xylene (o-xylene) - 13.3°C, meta-xylene (m-xylene) - 47.4°C , para-xylene (p-xylene) - 51°C.
- The boiling points of the isomers are as follows: ortho-xylene - 144.4°C , meta-xylene - 139.1°C , para-xylene - 138.3°C
- Xylene is insoluble in water but soluble in many organic solvents, such as ethanol, acetone, and ether.
- The vapour pressure of xylene varies with temperature and is higher than that of water.
- Xylene has a relatively low viscosity, making it flow easily.
- Xylene is highly flammable and can undergo combustion reactions in the presence of oxygen, producing carbon dioxide, water, and heat.

Chemical Properties:

- Xylene, like benzene and toluene, exhibits aromaticity due to its benzene ring structure, which consists of alternating double and single bonds. This structure makes xylene relatively stable and less reactive than aliphatic hydrocarbons.
- Similar to benzene and toluene, xylene undergoes substitution reactions rather than addition reactions due to its aromatic nature. Common substitution reactions include Nitration, Sulfonation, Halogenation, Alkylation/Acylation etc.
- **Oxidation Resistance**: Xylene is resistant to oxidation under normal conditions due to its aromatic stability. However, under more vigorous conditions, such as with strong oxidizing agents or high temperatures, xylene can undergo oxidation reactions to form various oxidation products, including carboxylic acids, phenols, and aldehydes.
- **Reactivity with Electrophiles**: Xylene, being an aromatic compound, readily reacts with electrophiles in electrophilic aromatic substitution reactions. This reactivity allows for the introduction of various functional groups onto the aromatic ring.

PRODUCTION OF BTX:

CATALYTIC REFORMING OF PETROLEUM NAPHTHA:

Catalytic reforming: A chemical process which is used to convert ***low-octane petroleum*** refinery naphtha into ***high-octane liquid products***; the product (reformates) are components of ***high-octane gasoline***; rearranging hydrocarbon molecules in a gasoline boiling range feedstock to produce other hydrocarbons having a higher antiknock quality; isomerization of paraffins, cyclization of paraffins to naphthenes, dehydrocyclization of paraffins to aromatics.The process also produces valuable byproducts like ***benzene***, ***toluene***, and ***xylene (BTX)***, which are essential raw materials for various chemical industries.

Process Steps:

1. Feedstock Preparation: The process begins with the preparation of a feedstock, typically low-octane petroleum refinery naphtha, which contains hydrocarbon derivatives with boiling points ranging between 60°C and 200°C (140°F–390°F). This feedstock is blended with hydrogen to facilitate the desired reactions.

2. Preparation: Before entering the catalytic reformer, the naphtha feed undergoes pre-treatment steps to remove impurities such as sulphur and nitrogen compounds. These impurities can deactivate the catalyst or lead to undesirable side reactions.

3. Exposure to Catalyst: The blended feedstock and hydrogen mixture is then exposed to a bifunctional catalyst, typically composed of platinum chloride or rhenium chloride, supported on a suitable carrier material such as alumina. The reaction typically takes place at temperatures ranging from 500°C to 525°C (930°F–975°F) and pressures ranging from 120 to 750 psi.

4. Reactions:

- **Isomerization of paraffins:** Straight-chain paraffins present in the feedstock are converted into branched-chain isomers, which have higher octane ratings.
- **Cyclization of paraffins to naphthenes:** Some of the paraffins are cyclized to form naphthenic compounds, which also contribute to the octane rating of the final product.
- **Dehydrocyclization of paraffins to aromatics:** Certain paraffinic hydrocarbons undergo dehydrogenation and cyclization to form aromatic compounds, including benzene, toluene, and xylene isomers (BTX).

5. Product Separation:

- The reformate product obtained from the catalytic reactor contains a mixture of hydrocarbons, including the desired aromatic compounds (BTX), as well as unreacted feedstock and other byproducts. The reformate is then subjected to separation processes to isolate the aromatic compounds from the other components.
- **Extraction:** A solvent extraction process, often utilizing solvents like diethylene glycol or sulfolane, is employed to extract the aromatic compounds from the reformate mixture.
- **Distillation:** The extracted aromatics are then subjected to distillation to separate them into individual components, namely benzene, toluene, and xylene isomers.

6. Final Product Recovery: Benzene, toluene, and xylene isomers obtained from the distillation process are collected as the final products. These aromatic compounds are crucial feedstocks for various industries, including petrochemicals, plastics, textiles, and pharmaceuticals.

7. Catalyst Regeneration: The catalyst used in the process undergoes deactivation over time due to coke deposition and other factors. Therefore, a portion of the catalyst is continuously regenerated to maintain its activity and efficiency in promoting the desired reactions.

Chemical Reactions associated with the above process:

- **Benzene Formation:**
  - Dehydrogenation of cyclohexane :

    $$C_6H_{12} \rightarrow C_6H_6 + 3H_2$$
- **Toluene Formation:**
  - Dehydrogenation of Methylcyclohexane:

$$C7H14 \rightarrow C7H8 + 3H2$$

❖ Isomerization of Xylene:

$$C_8H_{10} \rightarrow C_7H_8 + CH_4$$

- **Xylene Formation:**

❖ Dehydrogenation of Ethylbenzene:

$$C_8H_{10} \rightarrow C_8H_8 + H_2$$

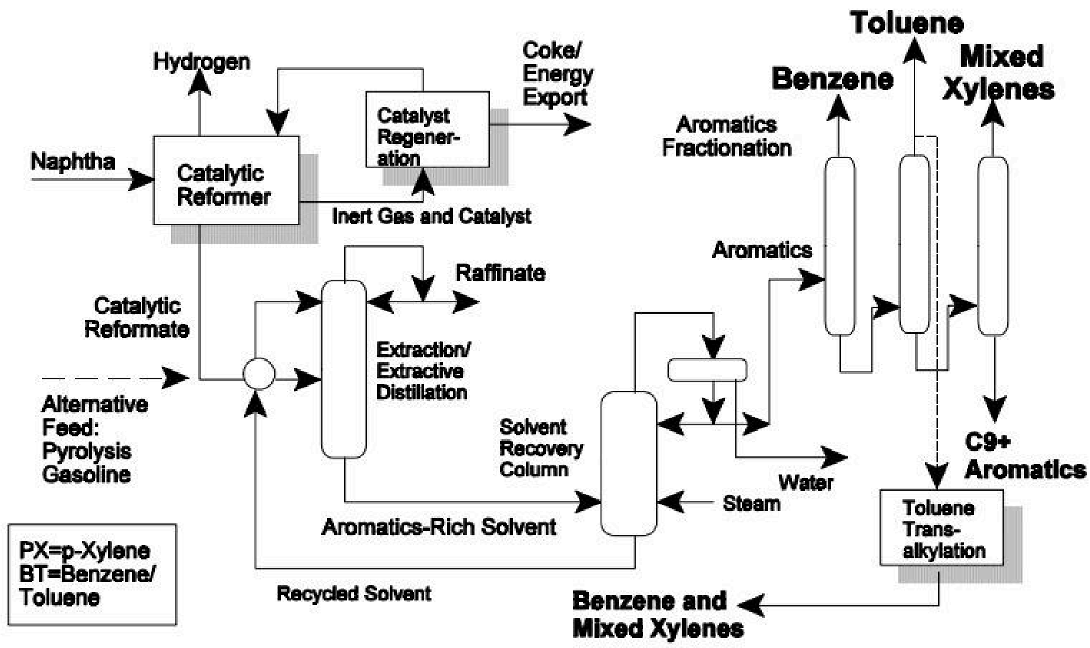
❖ Isomerization of Ethylbenzene to form ortho-, meta-, and para-xylene:

$$C_8H_{10} \rightarrow C_8H10$$

❖ Methylation of Toluene:

$$2C_7H_8 + C_2H_4 \rightarrow C_8H_{10} + C_2H_6$$

Schematic Diagram for Process:



STEAM CRACKING OF HYDROCARBONS:

Steam Cracking: Steam cracking is a ***high-temperature*** chemical process used in the petrochemical industry to thermally decompose hydrocarbon feedstocks, typically gaseous or light liquid hydrocarbons such as naphtha, into ***lower molecular weight products*** in the presence of ***superheated steam***.

Process Steps:

1. **Feedstock Preparation:** The process begins with the selection and preparation of a suitable feedstock, typically gaseous or light liquid hydrocarbons derived from petroleum, such as naphtha. Naphtha is a mixture of hydrocarbons with boiling points ranging from approximately 30°C to 200°C.

2. **Feedstock Dilution with Steam:** The hydrocarbon feedstock is diluted with superheated steam to facilitate the cracking reactions and control the reaction temperature. The steam also helps to prevent the formation of carbonaceous deposits on the reactor walls.

3. **Heating in Furnace:** The diluted feedstock is then introduced into a high-temperature furnace, where it is rapidly heated to temperatures typically ranging from 750°C to 950°C (1380°F–1740°F). This extreme heat is necessary to initiate the cracking reactions.

4. **Cracking Reactions:** Within the furnace, the heated hydrocarbon molecules undergo thermal decomposition, breaking apart into smaller fragments due to the high temperature and absence of oxygen. This process, known as cracking, results in the formation of lower molecular weight hydrocarbons, including unsaturated compounds such as ethylene, propylene, butylenes, benzene, toluene, xylenes, and ethylbenzene.

5. **Quenching and Product Separation**:

- After the cracking reactions have occurred, the hot cracked gas mixture is quickly quenched by passing it through a transfer line exchanger. This rapid cooling stops the cracking reactions and prevents further undesired side reactions.
- The cooled gas mixture, containing a variety of hydrocarbons including BTX, is then subjected to separation processes to isolate the desired products. This separation may involve techniques such as fractional distillation, solvent extraction, or other purification methods.

6. **Product Recovery:** The separated BTX products, namely benzene, toluene, and xylene isomers, are recovered as final products. These aromatic compounds are crucial feedstocks for various industries, including petrochemicals, plastics, textiles, and pharmaceuticals.

Chemical Reactions associated with the above process:

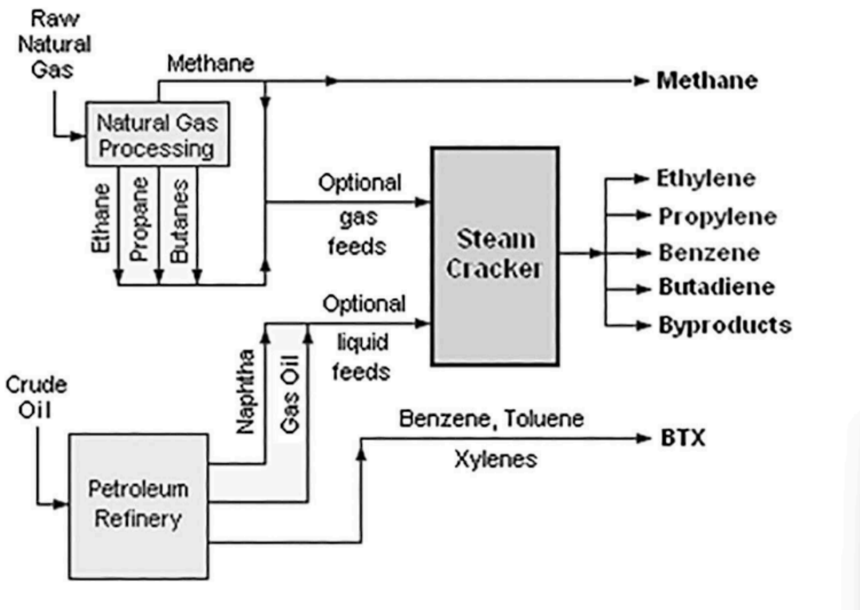
- **Benzene Formation:**
  - Thermal Cracking of Cyclohexane:

    $$2C_6H_{12} \rightarrow C_6H_6 + C_6H_{14}$$
- **Toluene Formation:**
  - Thermal Cracking of Heptane:

    $$C_7H_{16} \rightarrow C_6H_5CH_3 + CH_4$$

- **Xylene Formation:**
    - Thermal Cracking of Octane:
    $C_8H_{18} \rightarrow C_6H_4(CH_3)_2 + C_2H_4$

Schematic Diagram of Process:



HYDRODEALKYLATION:

Hydrodealkylation is a chemical process used to convert alkyl aromatic compounds, such as toluene or alkylbenzenes, into their corresponding aromatic hydrocarbons, such as benzene. This process involves the removal of alkyl groups (usually methyl groups) from the aromatic ring through catalytic hydrogenation.**Hydrodealkylation is an important industrial process for the production of benzene.**

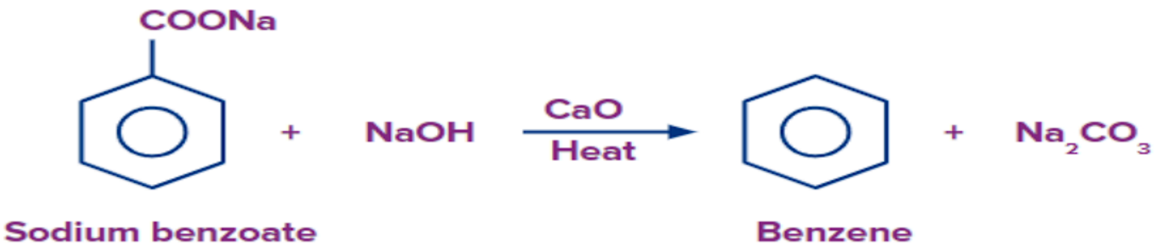
This reaction is catalysed by a suitable catalyst, often composed of metals like platinum, palladium, or other transition metals supported on a porous material like alumina or silica-alumina.
CHEMICAL REACTION:

- $C6H5CH3 + H_2 \rightarrow C6H6 + CH4$
- $C6H4(CH_3)2 + 2H2 \rightarrow C6H6 + 2CH4$

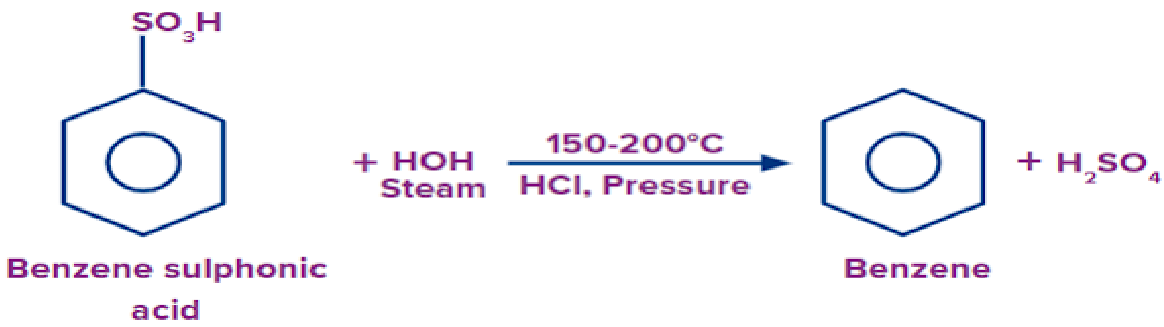
Hydrogen-rich makeup gas and recycle gas are compressed and combined with liquid alkyl aromatic feedstock. The combined feed undergoes preheating using heat exchange before entering the reactor. The reactor, which may contain a fixed bed catalyst, either tubular and non-catalytic, facilitates the process. After cooling, the effluent is separated into gas and liquid fractions, with a major portion of the gas recycled. The liquid fraction is then stripped of residual gas and fractionated to produce high-purity benzene and recycle alkyl aromatics. Yields range from **95-98%** for toluene conversion to benzene.

OTHER PROCESSES FOR PRODUCTION OF BENZENE:

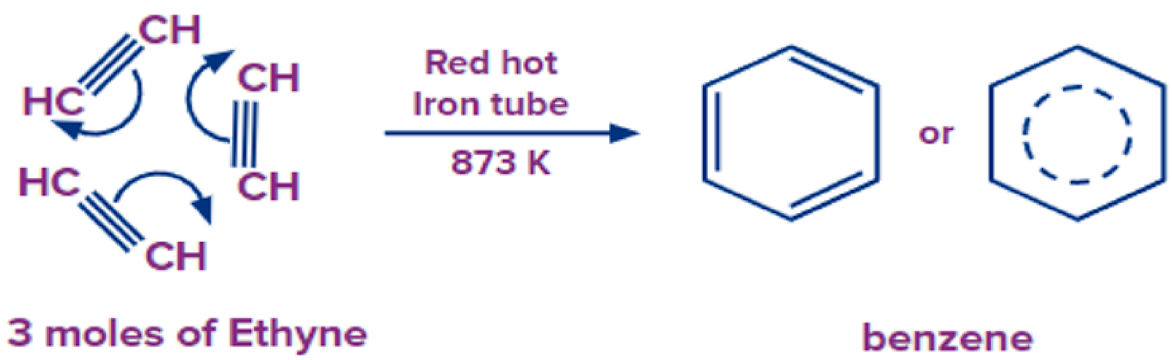
1. Preparation of benzene from Aromatic acid: In this process, the sodium salt of benzoic acid (sodium benzoate) is heated with soda lime to produce benzene and sodium carbonate.



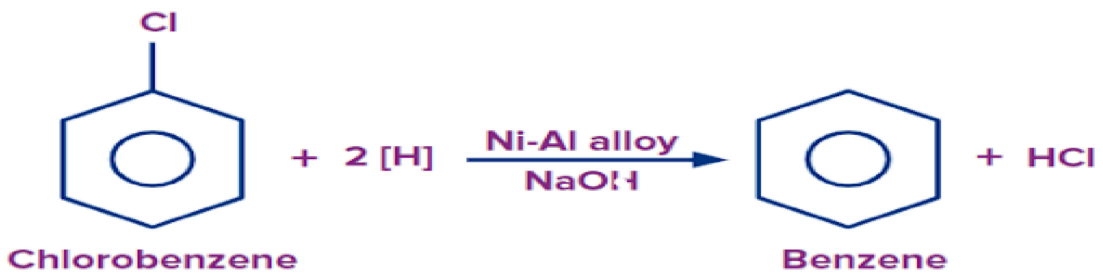
2. Synthesis of Benzene from Sulphonic Acids: Benzene sulfonate is treated with superheated steam to yield benzene and sulfuric acid.



3. Preparation of Benzene from Cyclic polymerisation of Alkynes: In this process, ethyne is passed through a red-hot iron tube at 873 K (600°C), where it undergoes cyclic polymerization to form benzene.



4. Preparation of Benzene from Chlorobenzene: Chlorobenzene on reduction with Ni-Al alloy and sodium hydroxide (NaOH) produces benzene.

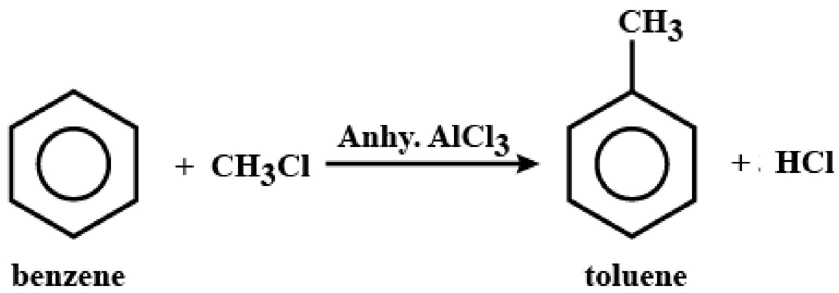


OTHER PROCESSES FOR PRODUCTION OF TOLUENE:

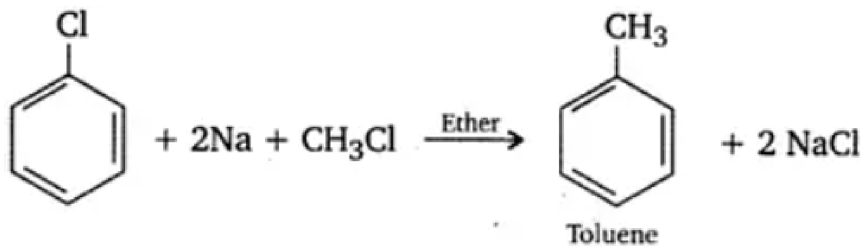
1)Steam Reforming: Methane, found in natural gas, can be steam reformed to generate synthesis gas (syngas), consisting of hydrogen and carbon monoxide. Syngas serves as a precursor for toluene production through processes like **Fischer-Tropsch synthesis** or other methods, facilitating the generation of diverse hydrocarbons.

2)Solvent Extraction: Solvent extraction to produce toluene involves mixing the toluene-containing mixture with a suitable solvent. Toluene selectively partitions into the solvent phase due to its higher solubility. After separation, toluene is recovered from the solvent phase through subsequent processing steps such as distillation or evaporation.

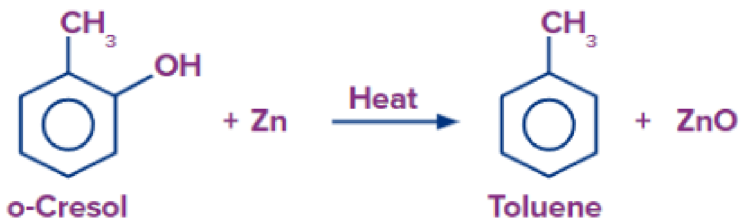
3)Friedel-Crafts Reaction: It involves the reaction of benzene with an alkyl halide in the presence of a Lewis acid catalyst, typically aluminum chloride (AlCl3).



4)Wurtz Fittig Reaction: When a mixture of chlorobenzene and methyl chloride reacts with sodium metal in the presence of dry ether solution yields Toluene as a major product.

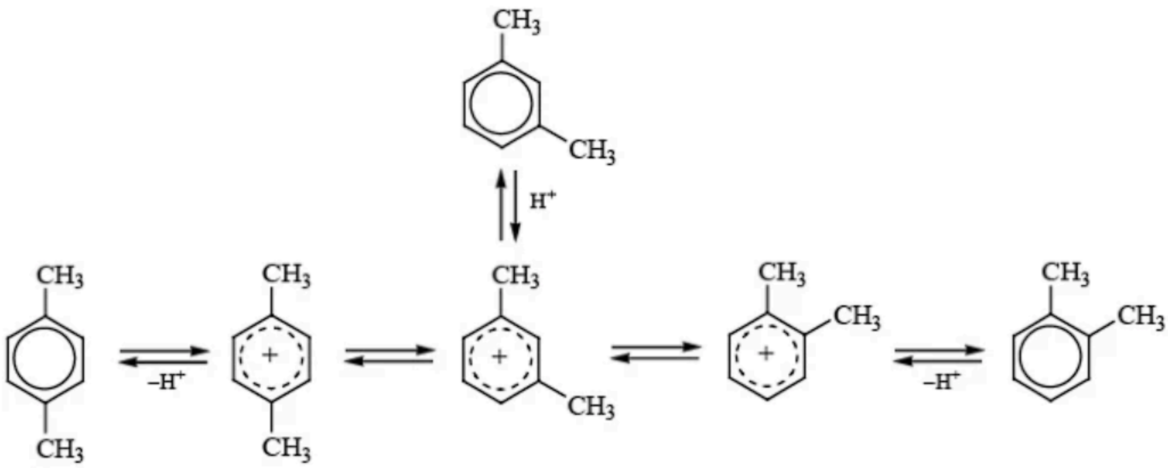


5)Distillation of Cresol and Zinc Dust:When ortho, meta, or para cresol is distilled with zinc dust, toluene is obtained.

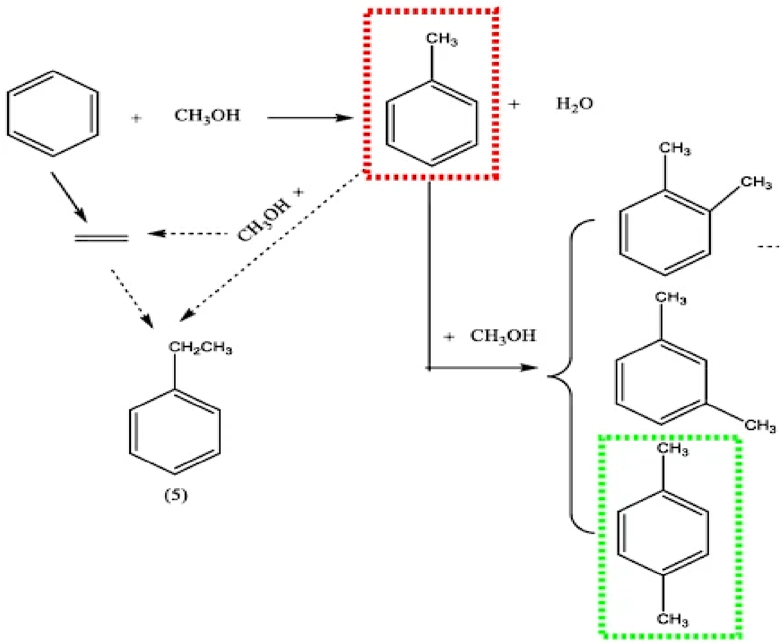


OTHER PROCESSES FOR PRODUCTION OF XYLENE:

1. Isomerisation: This process involves rearranging the molecular structure of the xylene isomers to increase the concentration of required xylene isomer.



2. Aromatic Alkylation: Xylene can also be synthesized through aromatic alkylation reactions, where benzene is alkylated with an alkylating agent, such as propylene, in the presence of a catalyst, typically zeolites or aluminium chloride. This process leads to the formation of various aromatic compounds, including xylene, as alkyl groups are added to the benzene ring.



APPLICATIONS OF BTX IN CHEMICAL INDUSTRIES:

1)BENZENE:

Benzene is a widely used Chemical and is a major part of gasoline. In the industries, it is majorly used:

- **As a Solvent**: Benzene is widely utilized as a solvent in diverse industrial, commercial, and research settings, facilitating the manufacture of chemical and plastic products, including resins and synthetic materials such as **nylon** and **Styrofoam**. Moreover, it plays a crucial role in the production of **asphalt**, essential for roofing and paving applications.
- The major usage of Benzene is for the production of **phenol** and **styrene** with the remaining for other aromatic derivatives such as **aniline , sulfonated detergents, DDT, maleic anhydride, chlorobenzene and cyclohexane.**
- Benzene is integral to tire and rubber production, adhesive formulation for shoe soles, and the manufacture of detergents, pesticides, herbicides, insecticides, and dyes.
- Due to the high octane number and natural availability, Benzene is used as a fuel.

2)TOLUENE:

- Toluene is used as a solvent in many consumer products and is used in paint thinners,rubber production,plastics, cements, nail polish remover, glues,detergents(Toluene sulfonates) and correction fluid.
- Toluene is used in the synthesis of many chemicals such as Benzoic Acid that is a precursor to phenol. It is also one of the key raw materials in the production of Toluene Diisocyanate which is an intermediate in the production of polyurethane foams.
- It is also used in the Dealkylation process with H2 to yield Benzene.
- It is also used in the production of Trinitrotoluene(TNT) which is used as an explosive.

3)XYLENE:

- Xylene is used as a raw material for the manufacture of fibres, dyes, and films.
- It is used as solvent for alkyd resins.
- It is used in laboratories to cool reaction vessels.
- It is used as a clearing agent.
- The chemicals derived from Xylene include:
    1. From Ortho-Xylene: **Phthalic Anhydride**, an acid competitive with naphthalene oxidation.

2. From Meta-Xylene: **Isophthalic Acid** which is competitive with phthalic acid for reinforced plastics and plasticizers.
3. From Para-Xylene: **Dimethyl Terephthalate** used in polyester fibers and films.

- It was used as a tear gas agent in **World War I**.

In summary, these chemicals have numerous industrial applications individually and collectively. These used can be summarised as:

1.**Solvent**: Toluene and xylene are widely used as solvents in various industries, including paint and coatings, adhesives, rubber, printing inks, and pharmaceuticals. Benzene, while less commonly used due to its toxicity, also has solvent properties.

2.**Feedstock for Chemical Synthesis**: Benzene, toluene, and xylene are important raw materials for the production of various chemicals. They serve as feedstocks in the synthesis of plastics, synthetic fibers (such as polyester and nylon), resins, detergents, pesticides, pharmaceuticals, and explosives (such as TNT - trinitrotoluene).

3.**Fuel Additive**: Toluene is sometimes used as an octane booster in gasoline. It improves the octane rating of gasoline and enhances engine performance.

4.**Aromatic Extracts**: Xylene is used in the production of aromatic extracts, which are used in the flavour and fragrance industry. These extracts are used in perfumes, cosmetics, soaps, and other consumer products.

5.**Rubber and Tire Manufacturing**: Toluene is used in the production of synthetic rubber, which is used in the manufacturing of tires, conveyor belts, hoses, and other rubber products.

6.**Cleaning Agent**: Toluene and xylene are used as cleaning agents in industrial processes, such as degreasing metal surfaces and cleaning electronic components.

7.**Dye and Paint Industry**: Xylene is used as a solvent and carrier in the dye and paint industry, where it helps dissolve pigments and improve paint viscosity.

8.**Laboratory Reagent**: Benzene, toluene, and xylene are used as reagents in various laboratory procedures, such as chromatography and extraction.

9.**Agricultural Applications**: Toluene is used in some agricultural applications, such as herbicides and insecticides formulations.

10.**Adhesives and Sealants**: Toluene is used as a solvent in the production of adhesives and sealants, providing good adhesion properties.

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