



## **Al-Mustaqbal University**

### **College of Engineering and Engineering Technologies**

#### **Department of Chemical Engineering and Petroleum Industries**

**Name of the substance:** Chemicals from petroleum

**Lecture number:** Five

**Lecture title :**

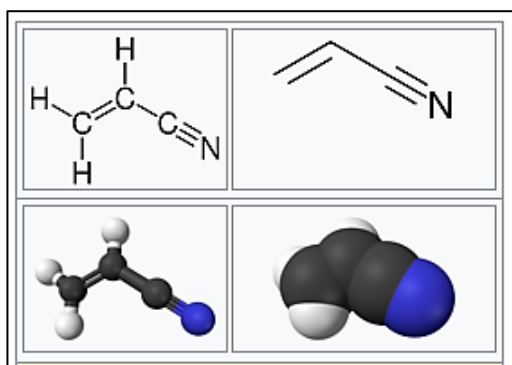
- Propylene derivatives
- Derivatives of  $c_4$  hydrocarbon
- Benzene derivatives
- Toluene derivatives
- Xylene derivatives
- Products of polymers(part 1)

Assist. Lec. Zainab Imad Abdul Sattar

## Propylene derivatives

### *Acrylonitrile:*

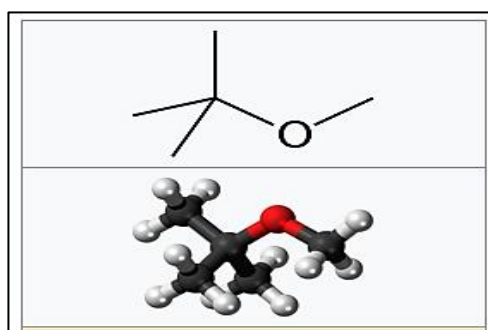
Acrylonitrile is an organic compound with the formula  $\text{CH}_2\text{CHCN}$  and the structure  $\text{H}_2\text{C}=\text{CH}-\text{C}\equiv\text{N}$ . It is a colorless, volatile liquid. It has a pungent odor of garlic or onions. Its molecular structure consists of a vinyl group ( $-\text{CH}=\text{CH}_2$ ) linked to a nitrile ( $-\text{C}\equiv\text{N}$ ). It is an important monomer for the manufacture of useful plastics such as polyacrylonitrile. It is reactive and toxic at low doses



## Derivatives of $\text{C}_4$ hydrocarbon

### *1. Methyl tert-butyl ether (MTBE):*

Methyl tert-butyl ether (MTBE), also known as tert-butyl methyl ether, is an organic compound with a structural formula  $(\text{CH}_3)_3\text{COCH}_3$ . MTBE is a volatile, flammable, and colorless liquid that is sparingly soluble in water. Primarily used as a fuel additive, MTBE is blended into gasoline to increase its octane rating and knock resistance, and reduce unwanted emissions.

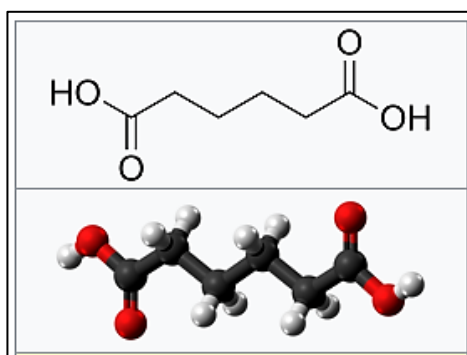


**Production and properties** : MTBE is manufactured via the chemical reaction of methanol and isobutylene. Methanol is primarily derived from natural gas, where steam reforming converts the various light hydrocarbons in natural gas (primarily methane) into carbon monoxide and hydrogen. The resulting gases then further react in the presence of a catalyst to form methanol. Isobutylene can be produced through a variety of methods. n-butane can be isomerized into isobutane which can be dehydrogenated to isobutylene. In the Halcon process, t-Butyl hydroperoxide derived from isobutane oxygenation is reacted with propylene to produce propylene oxide and t-butanol. The t-butanol can be dehydrated to isobutylene.

MTBE production in the U.S. peaked in 1999 at 260,000 barrels per day before dropping down to about 50,000 barrels per day and holding steady, mostly for the export market. After the purchase of SABIC, oil giant Saudi Aramco is now considered to be the world's largest producer with an estimated production capacity of 2.37 million metric tons per year (mt/yr). Worldwide production capacity of MTBE in 2018 was estimated to be 35 million metric tons

## 2. Adipic acid :

Adipic acid or hexanedioic acid is the organic compound with the formula  $(\text{CH}_2)_4(\text{COOH})_2$ . From an industrial perspective, it is the most important dicarboxylic acid: about 2.5 billion kilograms of this white crystalline powder are produced annually, mainly as a precursor for the production of nylon. Adipic acid otherwise rarely occurs in nature, but it is known as manufactured E number food additive E355. Salts and esters of adipic acid are known as adipates.



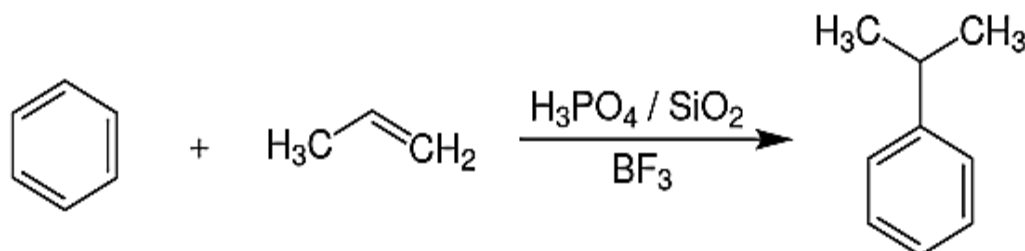
# Benzene derivatives

- 1- Ethyl benzene
- 2- Styrene
- 3- Nitrobenzene
- 4- Aniline
- 5- Cyclohexane
- 6- Cumene
- 7- Phenol
- 8- acetone

## 1. *Cumene*:

Cumene (isopropylbenzene) is an organic compound that contains a benzene ring with an isopropyl substituent. It is a constituent of crude oil and refined fuels. It is a flammable colorless liquid that has a boiling point of 152 °C. Nearly all the cumene that is produced as a pure compound on an industrial scale is converted to cumene hydroperoxide, which is an intermediate in the synthesis of other industrially important chemicals, primarily phenol and acetone (known as the cumene process)

**Production** Commercial production of cumene is by Friedel–Crafts alkylation of benzene with propylene. The original route for manufacturing of cumene was by alkylation of benzene in the liquid phase using sulfuric acid as a catalyst, but because of the complicated neutralization and recycling steps required, together with corrosion problems, this process has been largely replaced. As an alternative, solid phosphoric acid (SPA) supported on alumina was used as the catalyst.



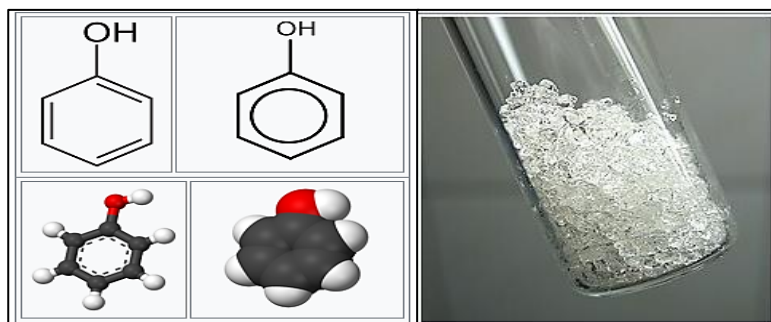
Since the mid-1990s, commercial production has switched to zeolite-based catalysts. In this process, the efficiency of cumene production is generally 70-75%. The remaining components are primarily polyisopropyl benzenes. In 1976, an improved

cumene process that uses aluminum chloride as a catalyst was developed. The overall conversion of cumene for this process can be as high as 90%. The addition of two equivalents of propylene gives diisopropylbenzene (DIPB). Using transalkylation, DIPB is comproportionated with benzene to give cumene.

## 2. Phenol :

Phenol, or Benzenol, (also known as carboic acid or phenolic acid) is an aromatic organic compound with the molecular formula  $C_6H_5OH$ . It is a white crystalline solid that is volatile. The molecule consists of a phenyl group ( $-C_6H_5$ ) bonded to a hydroxy group ( $-OH$ ). Mildly acidic, it requires careful handling because it can cause chemical burns.

Phenol was first extracted from coal tar, but today is produced on a large scale (about 7 million tonnes a year) from petroleum-derived feedstocks. It is an important industrial commodity as a precursor to many materials and useful compounds.[8] It is primarily used to synthesize plastics and related materials. Phenol and its chemical derivatives are essential for production of polycarbonates, epoxies, explosives, Bakelite, nylon, detergents, herbicides such as phenoxy herbicides, and numerous pharmaceutical drugs.



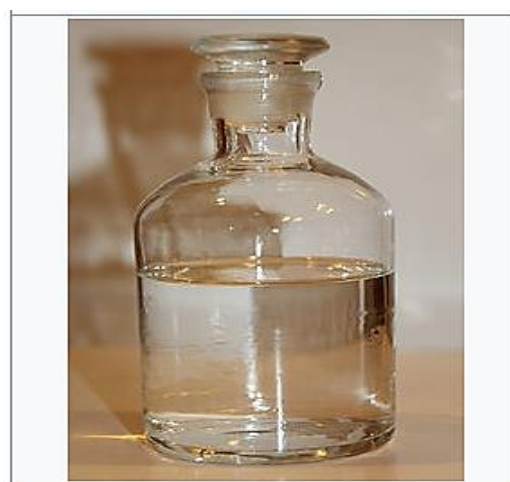
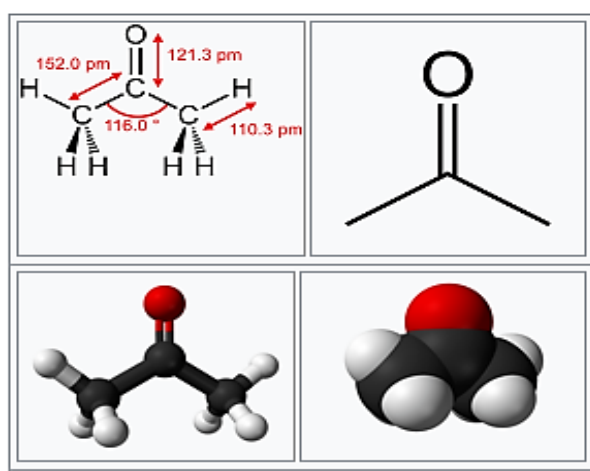
## 3. Acetone:

Acetone (2-propanone or dimethyl ketone) is an organic compound with the formula  $(CH_3)_2CO$ . It is the simplest and smallest ketone ( $>C=O$ ). It is a colorless, highly volatile and flammable liquid with a characteristic pungent odor.

Acetone is miscible with water and serves as an important organic solvent in industry, home, and laboratory. About 6.7 million tonnes were produced worldwide in 2010, mainly for use as a solvent and for production of methyl methacrylate and bisphenol A, which are precursors to widely-used plastics. It is a common building block in organic

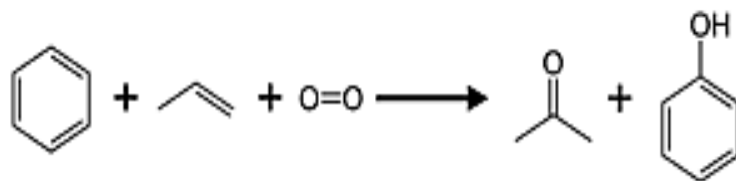
chemistry. It serves as a solvent in household products such as nail polish remover and paint thinner. It has volatile organic compound (VOC)-exempt status in the United States.

Acetone is produced and disposed of in the human body through normal metabolic processes. It is normally present in blood and urine. People with diabetic ketoacidosis produce it in larger amounts. Ketogenic diets that increase ketone bodies (acetone,  $\beta$ -hydroxybutyric acid and acetoacetic acid) in the blood are used to counter epileptic attacks in children who suffer from refractory epilepsy.



**Production** : In 2010, the worldwide production capacity for acetone was estimated at 6.7 million tonnes per year.[40] With 1.56 million tonnes per year, the United States had the highest production capacity, followed by Taiwan and mainland China. The largest producer of acetone is INEOS Phenol, owning 17% of the world's capacity, with also significant capacity (7–8%) by Mitsui, Sunoco and Shell in 2010. INEOS Phenol also owns the world's largest production site (420,000 tonnes/annum) in Beveren (Belgium). Spot price of acetone in summer 2011 was 1100–1250 USD/tonne in the United States

**Current method** : Acetone is produced directly or indirectly from propene. Approximately 83% of acetone is produced via the cumene process; as a result, acetone production is tied to phenol production. In the cumene process, benzene is alkylated with propylene to produce cumene, which is oxidized by air to produce phenol and acetone:

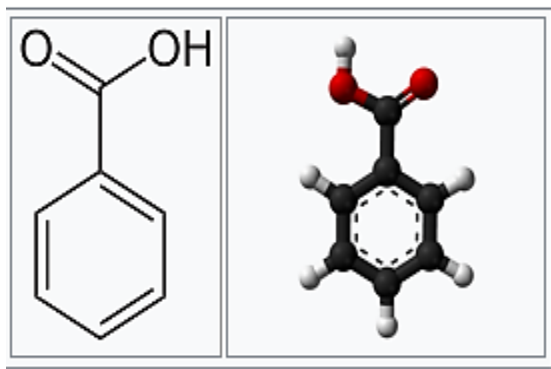


## Toluene derivativs

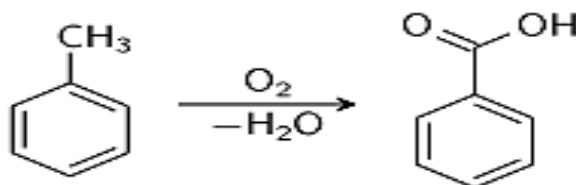
### *Benzoic acid*

Benzoic acid /ben'zou.ɪk/ is a white (or colorless) solid organic compound with the formula C<sub>6</sub>H<sub>5</sub>COOH, whose structure consists of a benzene ring (C<sub>6</sub>H<sub>6</sub>) with a carboxyl (–C(=O)OH) substituent. The benzoyl group is often abbreviated "Bz" (not to be confused with "Bn" which is used for benzyl), thus benzoic acid is also denoted as BzOH, since the benzoyl group has the formula –C<sub>6</sub>H<sub>5</sub>CO. It is the simplest aromatic carboxylic acid. The name is derived from gum benzoin, which was for a long time its only source.

Benzoic acid occurs naturally in many plants and serves as an intermediate in the biosynthesis of many secondary metabolites. Salts of benzoic acid are used as food preservatives. Benzoic acid is an important precursor for the industrial synthesis of many other organic substances. The salts and esters of benzoic acid are known as benzoates.



**Production :** Benzoic acid is produced commercially by partial oxidation of toluene with oxygen. The process is catalyzed by cobalt or manganese naphthenates. The process uses abundant materials, and proceeds in high yield.



The first industrial process involved the reaction of benzotrichloride (trichloromethyl benzene) with calcium hydroxide in water, using iron or iron salts as catalyst. The resulting calcium benzoate is converted to benzoic acid with hydrochloric acid. The product contains significant amounts of chlorinated benzoic acid derivatives. For this reason, benzoic acid for human consumption was obtained by dry distillation of gum benzoin. Food-grade benzoic acid is now produced synthetically.

## Xylene derivatives

### *Terephthalic acid:*

Terephthalic acid is an organic compound with formula C<sub>6</sub>H<sub>4</sub>(CO<sub>2</sub>H)<sub>2</sub>. This white solid is a commodity chemical, used principally as a precursor to the polyester PET, used to make clothing and plastic bottles. Several million tons are produced annually. The common name is derived from the turpentine-producing tree *Pistacia terebinthus* and phthalic acid.

### *Uses :*

- Polyester fibers based on PTA provide easy fabric care, both alone and in blends with natural and other synthetic fibers. Polyester films are used widely in audio and video recording tapes, data storage tapes, photographic films, labels and other sheet material requiring both dimensional stability and toughness.

- Terephthalic acid is used in paint as a carrier.



- Terephthalic acid is used as a raw material to make terephthalate plasticizers such as dioctyl terephthalate and dibutyl terephthalate.

- It is used in the pharmaceutical industry as a raw material for certain drugs.

- In addition to these end uses, Terephthalic acid based polyesters and polyamides are also used in hot melt adhesives.

- PTA is an important raw material for lower molecular weight saturated polyesters for powder and water-soluble coatings.

- In the research laboratory, terephthalic acid has been popularized as a component for the synthesis of metal-organic frameworks.

- The analgesic drug oxycodone occasionally comes as a terephthalate salt; however, the more usual salt of oxycodone is the hydrochloride.

- Pharmacologically, one milligram of hydrochloridum oxycodonae is equivalent to 1.13 mg of terephthalas oxycodonae.

- Terephthalic acid is used as a filler in some military smoke grenades, most notably the American M83 smoke grenade and M90 vehicle-employed smoke grenade, producing a thick white smoke that acts as an obscurant in the visual and near-infrared spectrum when burned.

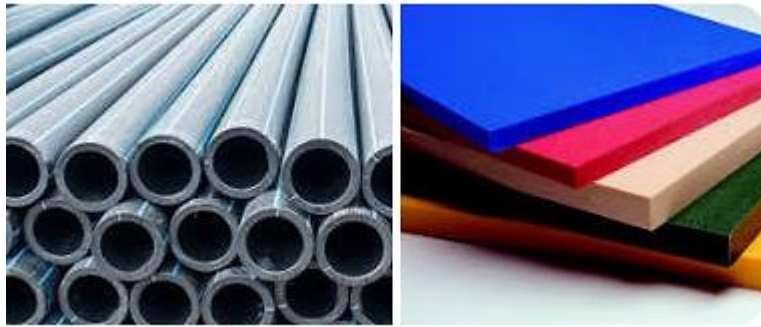
## *Products of polymers:*

- **LDPE:** LDPE is used for manufacturing various containers, dispensing and squeeze bottles, tubing, plastic parts of computer components, moulded laboratory equipment and many caps and closures. It is robust enough to be almost unbreakable.



Low-density polyethylene (LDPE) is a thermoplastic derived through the polymerization of ethylene using a high-pressure process. Low-density polyethylene resins typically have a density ranging from  $0.910 \text{ g/cm}^3$  to  $0.940 \text{ g/cm}^3$ . Its construction allows for excellent low tensile strength and high ductility making it ideal for the production of plastic bags, foam and packaging films as well as containers and packaging supplies. The high level of transparency of this material makes it ideal for the packaging industry. One of the world's few producers of low-density polyethylene, the company uses Luboutique technology to deliver superior grades of low-density polyethylene that are most suitable for film applications.

- **HDPE** : is an acronym for High Density Polyethylene. High Density Polyethylene is a polyethylene thermoplastic made from petroleum. HDPE is commonly recycled and made into composite wood or plastic lumber.



High-density polyethylene (HDPE) is one of the most widely used thermoplastic polymers, produced through the ethylene polymerization process. It is characterized by its good impact strength despite its low strength and resistance, and is also famous for its chemical resistance properties. High-density polyethylene has a typical density of over 0.941 g/cm<sup>3</sup> and is used to produce tubes, films, shopping bags, containers, drums, cans, caps, packing supplies, toys, etc. Its diverse properties make it popular in the packaging, construction, infrastructure, personal care, consumer and home care industries. Manufacturing uses the Advanced ACP process to manufacture high-density polyethylene. This technology is distinguished by being the most advanced version of the Hostalen technology used to produce multimedia high-density polyethylene resins used to produce pipe types and other grades.