

# Comprehensive Review on C5, C6 and C9 Chemicals – Production Processes, Applications and Market Analyses

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**Abstract:** A comprehensive study includes the major C5, C6 and C9 chains products and their derivatives. Each chemical product is described thoroughly by showing its chemical structure, industrial manufacturing processes (technologies), applications and market data. More details regarding some process technologies are mentioned to familiarize you with the operating conditions, used catalysts and licensors of each technology. Worldwide statistics showed that china is the dominant producer and consumer for DNT chemical where china supply and demand for DNT is about the half of the total worldwide production and consumption capacities.

**Index Terms**— Chemicals, C5 chain, Technologies, Applications, Market, Petrochemical.



## **1. Introduction**

Petrochemical industry is becoming more dominant than oil and gas companies due to the fact that the profits of petrochemical plants are much higher than petroleum based refineries. Understanding the new process technologies of valued chemicals will allow us to select the most convenient profitable rout for each substance. Additionally, being familiar with each chemical demand/supply, structure and applications is very important in petrochemical business.

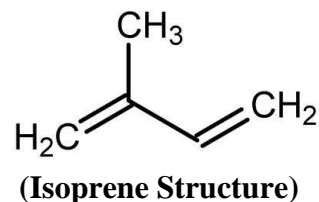
## **2. Isoprene**

### **2.1 Chemical Structure**

2-methyl-1,3-butadiene, which is a common organic compound with the formula  $\text{CH}_2=\text{C}(\text{CH}_3)\text{CH}=\text{CH}_2$ . It is a colorless volatile liquid. Isoprene is the monomer used for the production of synthetic rubbers called polyisoprenes.

## 2.2 Isoprene Derivatives

- I. CIS-Polyisoprene Rubber (PIR)
- II. Styrene-Isoprene-Styrene (SIS)
- III. Butyl Rubber (BR)
- IV. SEPS\*



\* SEP/SEPS are thermoplastic elastomers which consist of varied amounts of polyisoprene (EP) and polystyrene (S) combined in di-block (SEP) or tri-block (SEPS) copolymers.

Various isoprene products developed by **Kuraray** are displayed as a branching Isoprene Tree as new & more products are created in **Figure 1**.

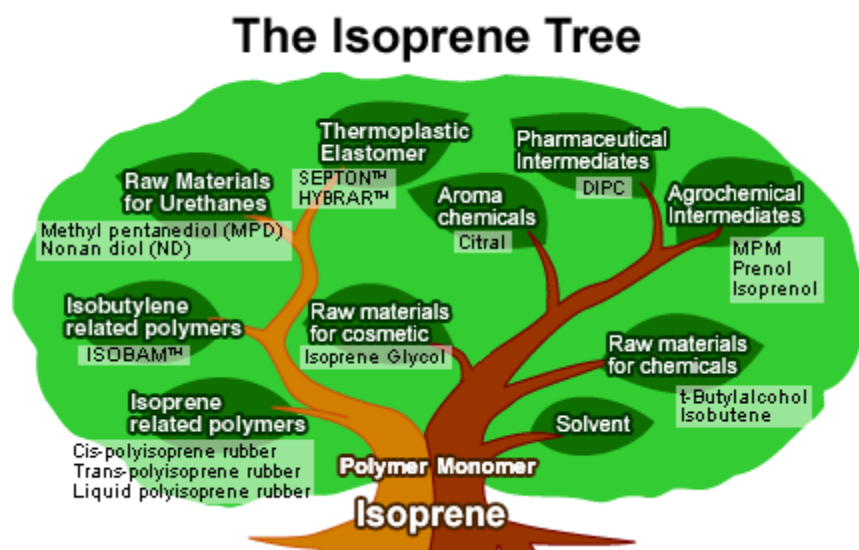


Figure 1 – Isoprene Products Shown by The Isoprene Tree

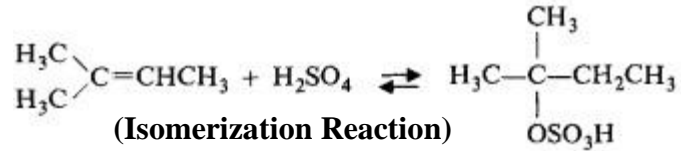
## 2.3 Industrial Production Processes (Routes)

- 1- Extraction from C5 Stream
- 2- Isopentane Dehydrogenation
- 3- Isobutylene Carbonylation
- 4- Acetylene-Based
- 5- Isoamylene Dehydrogenation
- 6- MTBE Oxidation
- 7- Dehydration of 2-methylbutanal

### 2.3.1 Dehydrogenation processes with isopentane and isopentenes

1. The feedstocks are the C<sub>5</sub> fractions from catalytic cracking processes
2. Alkenes are dehydrogenated before the alkanes.
3. Then, a subsequent purification for the separation of 1,3-pentadiene (piperylene),
4. Therefore, Shell first separates the 2-methylbutenes from the rest of the C<sub>5</sub> products in a so-called Sinclair extraction with 65% H<sub>2</sub>SO<sub>4</sub>.

5. The acid initially isomerizes the mixture of the 2-methylbutenes mainly to 2-methyl-2-butene, and then adds to form the sulfuric acid ester:



6. The ester is then split at 35 °C and the C<sub>5</sub> olefin is extracted.  
 7. **The last step, required dehydrogenation to isoprene** is similar to processes for butadiene.

**Table 1 - Isopentane Dehydrogenation Process Data**

<b>Process Name</b>	The Shell process
<b>Feedstock</b>	C <sub>5</sub> naphtha cracking fractions
<b>Catalyst</b>	Fe <sub>2</sub> O <sub>3</sub> - Cr <sub>2</sub> O <sub>3</sub> - K <sub>2</sub> CO <sub>3</sub>
<b>Temperature</b>	600 °C
<b>Yields</b>	about 85%
<b>Product</b>	Pure isoprene (99.0-99.5 wt%)*
<b>Licensor</b>	Shell, ArcO and Exxon

\* It is isolated by extractive distillation with acetonitrile.

### 2.3.2 Extraction from C5 stream

Isoprene is commonly produced by extraction of the isoprene molecule from Crude C5 mixtures such as the C5 Diene Crude product. During this extraction process piperylene is also concentrated and collected as product from which the C5 based resin can be produced. The cyclopentadiene often found in the raw material can be dimerized to form dicyclopentadiene (DCPD)

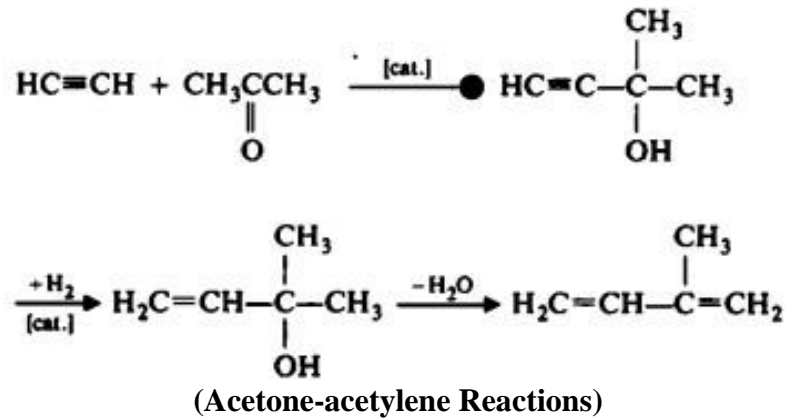
The process starts from a fluid catalytically cracked initial C5 fraction, a final C5 fraction which is enriched with isoprene and purified and usable to form a medium for the selective polymerization of isoprene in the presence of a catalytic system based on a conjugated diene. The basic concept is about separating the isoprene, 1,3-pentadiene and dicyclopentadiene from a C5 cuts low investment and energy consumption required leads to reduction in the operation cost and the production cost. See **Table 2** for more details.

**Table 2 - Extraction from C5 Stream Process Data**

<b>Process Name</b>	“FCC” initial C5 fractions	
<b>Distillation</b>	Extraction or Azeotropic distillation	
<b>Feedstock</b>	C <sub>5</sub> Stream	
<b>Catalyst</b>	-	
<b>Temperature</b>	60-150° C	
<b>Pressure</b>	1.0-1.5 MPa	
<b>Yields</b>	-	
<b>Products</b>	Name	Wt. %
	Isoprene (with purity > 99.3%)	14 – 18%
	Piperylene	10 – 20%
	Cyclopentadiene	8 – 19%
	Dicyclopentadiene (DCPD)	0 – 5%
<b>Licensor</b>	-	

### 2.3.3 Acetylene-Based Process

The acetone-acetylene process was developed by Snamprogetti, and was used in a 30000 tonne-per-year plant in Italy until 1982. In the first step,



Refer to **Table 3** for more details about the above reactions sequentially.

**Table 3 - Acetylene-Based Process Data**

<b>Process Name</b>		acetone-acetylene process	
<b>Feedstock</b>		Acetone & acetylene	
<b>Process Description</b>	<b>Step (1)</b>	<i>Acetone-acetylene reaction in liquid ammonia</i>	
		<b>Catalyst</b>	KOH
		<b>Temperature</b>	10-40°C
		<b>Pressure</b>	20 bar
		<b>Product</b>	Methylbutynol
	<b>Step (2)</b>	<i>Methylbutynol is hydrogenated to Methylbutenol</i>	
	<b>Step (3)</b>	<i>Dehydration of methylbutenol</i>	
		<b>Catalyst</b>	Al <sub>2</sub> O <sub>3</sub>
		<b>Temperature</b>	250-300°C
		<b>Pressure</b>	Atmospheric
	<b>Final Product</b>	Isoprene	
<b>Selectivity</b>		Overall selectivity to isoprene is 85%	

### 2.3.4 Isoamylene Dehydrogenation Process

Isoprene also produced from the dehydrogenation of Isoamylene compounds which contains at least two isoamylene monomers (2-methyl 2-butene and 2-methyl 1-butene) also there is a much lower amounts of 3-methyl 1-butene. However, dehydrogenation reaction occurred in the presence of oxygen and provided by adding steam to the reaction zone. Isoamylene dehydrogenation process required high steam-to-hydrocarbon ratios (10:1 at least). The feedstock of Isoamylene and steam are contacted with a catalyst (Consists of ferric oxide and potassium) in the within the reactor under a vacuum at a pressure of 1000 mbar or less. The operating temperature is 300°C at least with the conversion of 30%. More data is shown in **Table 4** below.

**Table 4 - Isoamylene Dehydrogenation Process Data**

<b>Process Name</b>	Isomylene Dehydrogenation
<b>Feedstock</b>	Isoamylene with steam
<b>Catalyst</b>	Ferric oxide and potassium
Steam-to-Hydrocarbon	Oxygen is provided by adding steam in this ratio steam-to-hydrocarbon ratios (10:1 at least)
<b>Temperature</b>	above 600° C
<b>Pressure</b>	1000 mbar or less
<b>Conversion</b>	30% at least
<b>Product</b>	Isoprene

### 2.3.5 MTBE Oxidation Process

In this process the reaction is done in a series of two reactors which contain the two functionally different catalysts, isoprene is produced by passing the mixture of MTBE (methyl-tert-butyl ether), air and steam over bi-functional acid and oxidation catalyst which cracks MTBE to isobutylene and methanol, and oxidizes the methanol to formaldehyde in the first reactor. Then, in second reactor, another mono-functional acidic catalyst catalyzes the reaction of formaldehyde with isobutylene to form isoprene.

**Table 5 - MTBE Oxidation Process Data**

<b>Process Name</b>	MTBE Oxidation Process	
<b>Feedstock</b>	MTBE, air and steam	
<b>Catalyst</b>	bi-functional	mono-functional
	Acid & oxidation	Acidic catalyst
<b>Temperature</b>	200 - 350 °C	
<b>Pressure</b>	Atmospheric	
<b>Yields</b>	about 85%	
<b>Product</b>	Isoprene	

### 2.3.6 Dehydration of 2-methylbutanal Process

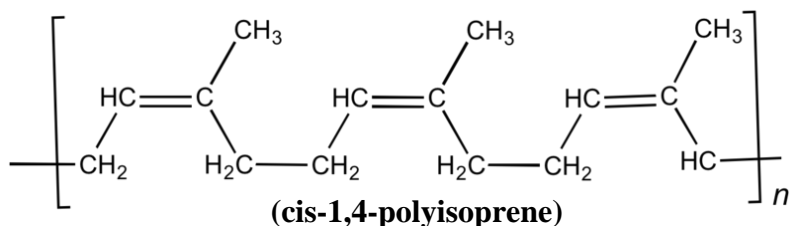
Using the process, dehydration of the corresponding carbonyl compound having the same number of carbon atoms, isoprene may be prepared from 2-methylbutanal at a temperature of 300° to 450°C using a catalyst comprising aluminium phosphate having the cristobalite structure. Look at **Table 6**.

**Table 6 - Dehydration of 2-methylbutanal Process Data**

<b>Process Name</b>	Dehydration of 2-methylbutanal
<b>Feedstock</b>	2-methylbutanal
<b>Catalyst</b>	aluminium phosphate
<b>Temperature</b>	300 - 450°C
<b>Product</b>	isoprene
<b>Licensors</b>	Goodyear Tire & Rubber

## 2.4 Worldwide Statistics

- About 800,000 tons are produced annually.
- 95% of isoprene production is used to produce cis-1,4-polyisoprene ;a synthetic rubber.



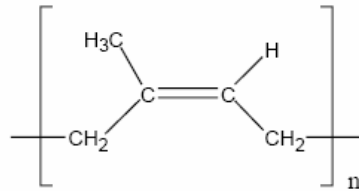
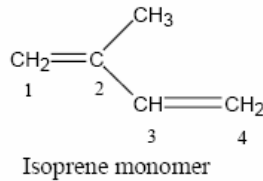
## 2.5 Applications

They are used in a wide variety of rubber applications such as Medical equipment, baby bottle nipples, toys, shoe soles, tires, elastic films and threads for golf balls or textiles. Other uses include adhesives, paints and coatings. Also, it is used in applications such as in inner tubes. Styrene-isoprene rubber is a copolymer that is used in pressure sensitive adhesives.

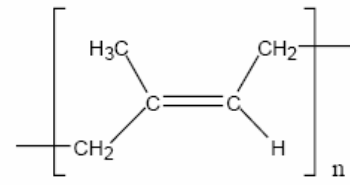
## 3. Polyisoprene Rubber (PIR, PI or IR)

### 3.1 Chemical Structure

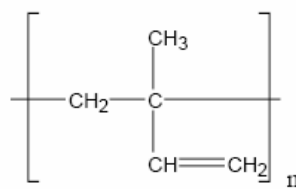
The polymerization of isoprene monomer can proceed in a 1,2-, 3,4-, or 1,4- mode to give the structures shown below.



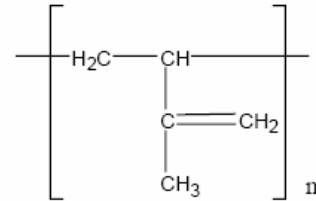
cis-1,4-addition



trans-1,4-addition



1,2-addition



3,4-addition

### 3.2 Manufacturing Process (cis-1,4-Polyisoprene Rubber)

Figure on the next page, gives a simplified flow diagram for an isoprene polymerization process. Before entering the reactors, the solvent, catalyst, and isoprene monomer must be free of chemical impurities, moisture, and air—all of which are catalyst poisons. The purified streams first enter a chain of reactors in series into which the catalyst is injected, and the polymerization begins

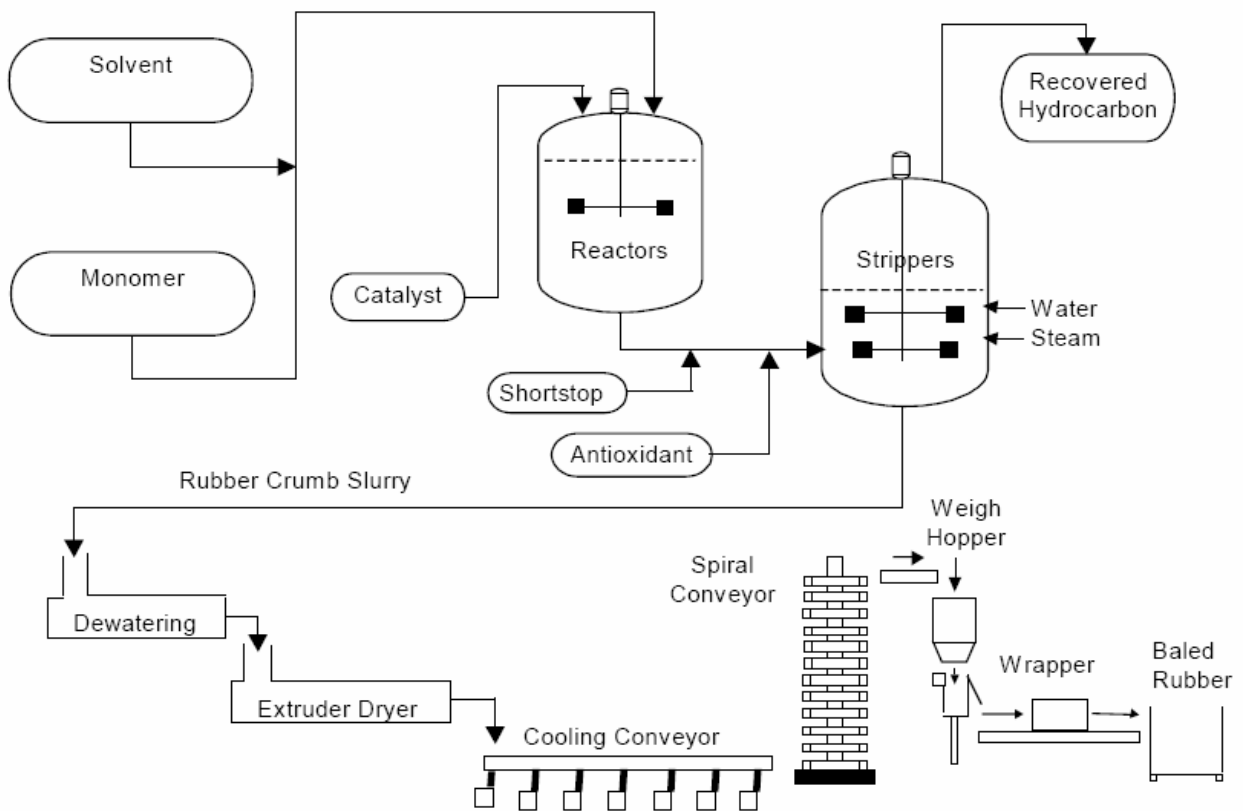
After the desired extent of polymerization has been attained, a short stop or catalyst deactivator is added to the cement so no further linkage of monomer or polymer takes place. A non-staining antioxidant is then added to protect the polymer during finishing and storage.

In the next step, the cement mixture is put through a stripping operation whereby the solvent is recovered and the polymer cement converted to a crumb by hot water and steam. The crumb slurry is processed through extruders to remove water before it is cooled, baled, packaged, and placed in storage ready for shipment. See **Table 7** for the types of catalysts and the production process shown in **Figure 2**.

**Used Catalyst: (Table 7)**

**Table 7 – Types of Catalysts Used for IR Production Process**

Symbol	Ti-IR	Li-IR
<b>Catalyst Name</b>	Ziegler-Natta (Titanium-aluminum)	Lithium-aluminum
<b>Struc.</b>	<b>Cis- 1,4</b>	98.5%
	<b>Trans- 1,4</b>	1%
	<b>3,4</b>	0.5%
<b>Rubber content</b>	> 99%	> 99%
<b>Producer</b>	Goodyear	Kuraray



**Figure 2 – IR Production Process**



### 3.3 Applications

- Applications in industries require low water swell
- High gum tensile strength, good resilience, high hot tensile and good tack.
- Gum compounds based on synthetic polyisoprene are being used in rubber bands, cut thread, baby bottle nipples, and extruded hose.
- Black loaded compounds find use in tires, motor mounts, pipe gaskets, shock absorber bushings and many other molded and mechanical goods.
- Mineral filled systems find applications in footwear, sponge, and sporting goods.
- Polyisoprene *Market applications* include;

#### *Medical*

- Surgical gloves
- Catheters
- Tube connectors
- Needle shields
- IV bag and medical bottle stoppers
- Cohesive bandages

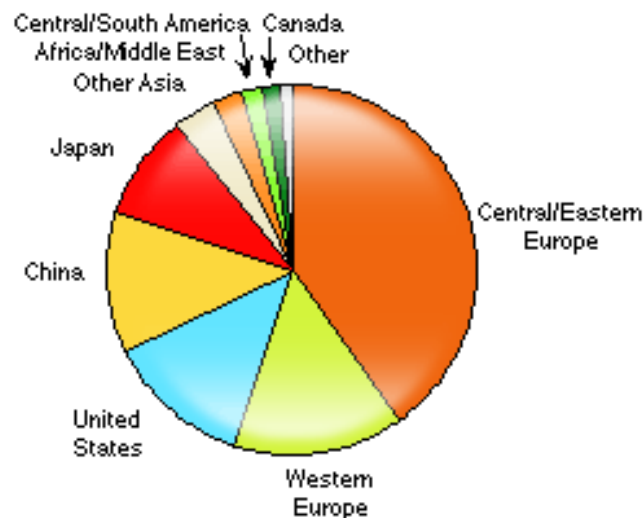
#### *Consumer and Industrial*

- Electronics
- Condoms
- Footwear
- Food packaging adhesives
- Paint additives
- Resins

### 3.4 Market Data

- **Tires and tire products accounted for about 75% of world polyisoprene consumption in 2010**, and over 90% of the consumption in Central & Eastern Europe.
- The following pie chart (**Figure 3**) shows world consumption of IR elastomers:

**World Consumption of Polyisoprene Elastomers—2010**



**Figure 3 – IR Elastomers World Consumption on 2010**

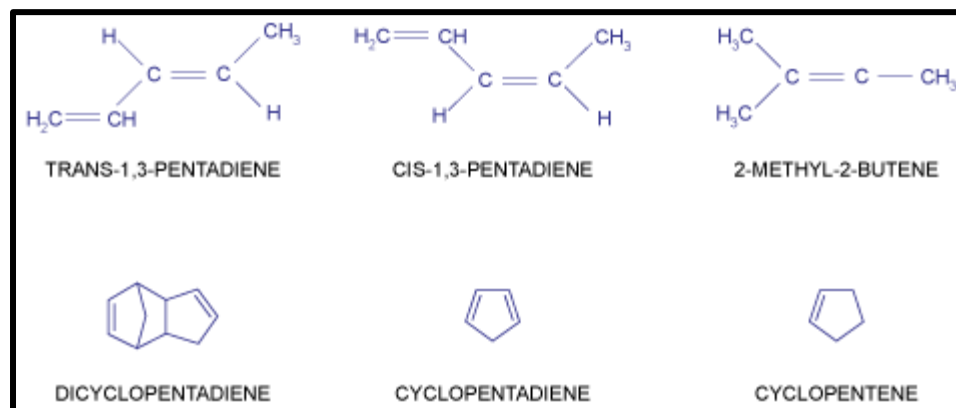
- **Russia is and will continue to be the world market leader** in terms of capacity, production and exports.
- **China has the highest average annual consumption growth rate** and has increased its consumption
- The Central and Eastern European region (mostly **Russia**) will continue to be **the largest consumer of polyisoprene**.
- **World polyisoprene elastomer consumption is expected to grow at nearly 4% per year to 2015**, driven mainly by China, Central and Eastern Europe, and other developing countries.

## 4. C5 Resins

### 4.1 Chemical Structure

C5 resins are thermoplastic resins, obtained from polymerizing unsaturated aliphatic petroleum feedstock. Aliphatic Resins are produced from the liquid C5 piperylene feedstock and can be polymerized to a hard resin using a Lewis acid catalyst by selecting an appropriate temperature and pressure to obtain the desired softening point and molecular weight

**Figure 4** below illustrates that C5 piperylene is the basic raw material for aliphatic tackifiers and contains various monomers.



**Figure 4 - C5 Piperylene Hydrocarbon Resin Oil Composition**

### 4.2 Manufacturing Process

Resin technology is based mainly on Lewis acid catalyzed/cationic polymerization (Catalytic Process) and can be followed by hydrogenation to improve properties such as a color and saturation.

C5 resins produced from feed blends comprising: isoprene; piperylene (PIPS); aromatic olefins; cyclopentadiene and dicyclopentadiene.

### 4.3 Applications

- Assembly, asphalt modification, roofing, road paving and modified wax compounds
- Pressure sensitive adhesives tapes & labels, hot melt adhesives for nonwoven product
- Paint and coatings applications and printing inks
- Rubber compounding

### 4.4 Market Data

- Global petroleum resins market is forecast to reach 2.59 Million Tons by the year 2017.
- The synthetic resin market as a whole (C5 and C9), is growing at around 3.6 percent per year on average.
- The petroleum resins market worldwide is traditionally dominated by western markets of Europe and North America.
- The Chinese petroleum resin market is currently dominated by domestic players. The continued growth of petroleum resin market in China has attracted the attention of Western manufacturers, such as ExxonMobil and Eastman, which recently established facilities in the country.
- Major geographic markets including the United States, Canada, Japan, Europe, Asia-Pacific, Middle East and Latin America.
- ExxonMobil Chemical is the world leader in synthetic resins in this increasingly global business, other major producer includes Hercules, Neville, Eastman and Nippon Zeon.

## 5. Benzene/Toluene and Xylene (BTX)

### 5.1 Chemical Structure

It is mixtures of Benzene, Toluene and Xylene isomers, all aromatic hydrocarbons.

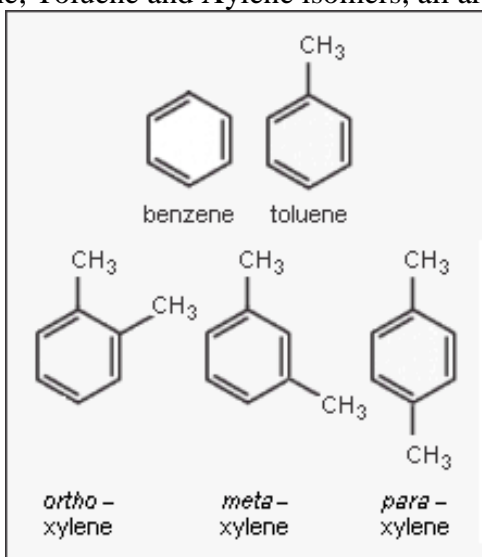


Figure 5 – BTX Chemical Structures

## 5.2 Manufacturing Process

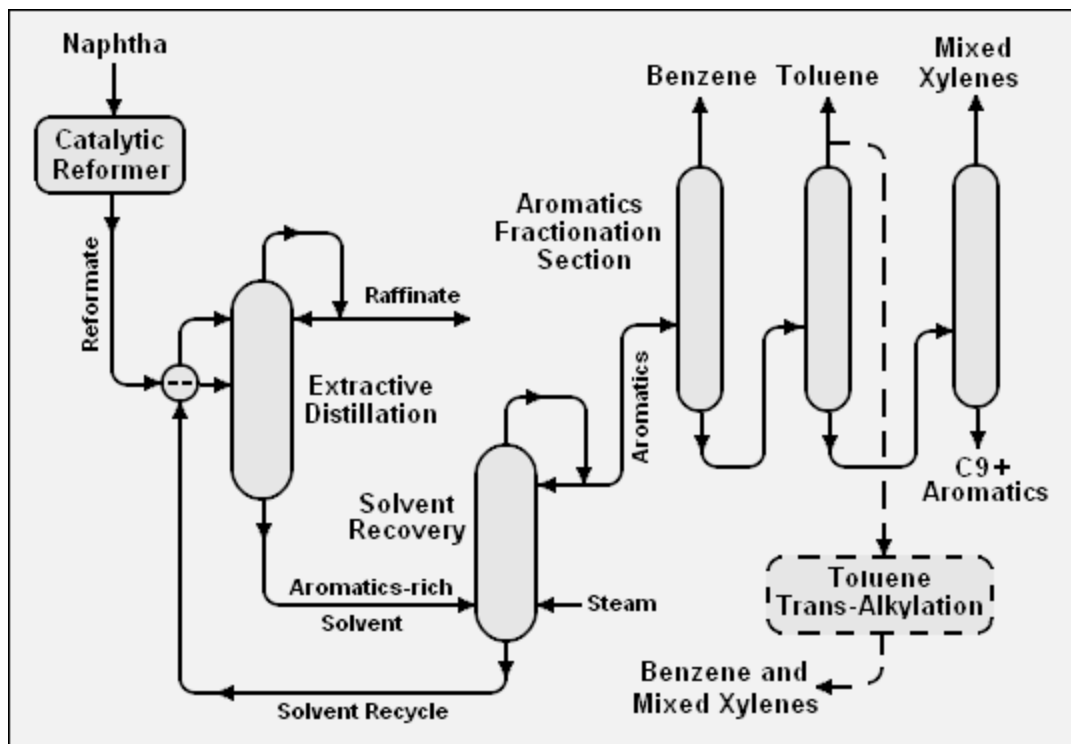
### 5.2.1 Two Process Routes

The manufacturing process of BTX is shown in **Table 8**, below.

**Table 8 – BTX Production Processes**

BTX production Process	Catalytic Reforming	Steam Cracking
<b>Feedstock</b>	Naphtha (C6 to C11, C12)	Naphtha (C6 to C11, C12)
<b>Products</b>	<i>Reformate</i> product containing C <sub>6</sub> to C <sub>8</sub> aromatics (benzene, toluene, xylenes) as well as paraffins and heavier aromatics containing 9 to 11 or 12 carbon atoms.	<i>Pygas</i> - pyrolysis gasoline (C <sub>6</sub> to C <sub>8</sub> & C <sub>9</sub> to C <sub>12</sub> ) and non-aromatic (C <sub>6</sub> ) cyclic hydrocarbons (naphthenes)
<b>Main product</b>	xylenes and toluene are the main components	Pygas is typically rich in benzene
<b>Global production percent</b>	70% of the global production of benzene is by extraction from either reformate or pyrolysis gasoline	
<b>BTX extraction process</b>	Use of a solvent either for liquid-liquid extraction or extractive distillation	

**Figure 6** is a schematic flow diagram of catalytic reforming method, involving extractive distillation, for extraction of the BTX aromatics from a catalytic reformate:



**Figure 6 – Extraction of BTX from a Catalytic Reformate**

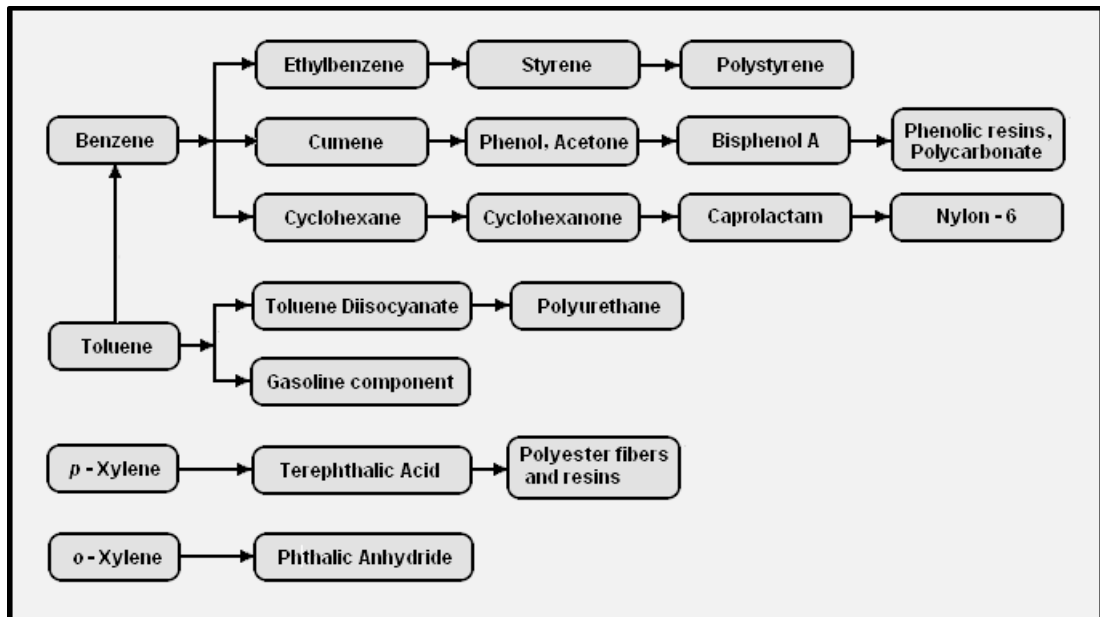
### 5.2.2 Technology Licensors

There are two major licensors of aromatics technology, namely UOP and IFP.

- **UOP** has developed a new family of zeolites that can be used in alkylation of aromatics, isomerization of aromatics and alkylation of isoparaffins.
  - Modern catalytic reforming using platinum, commercialized by UOP
- **IFP** has discovered a catalyst with substantially improved properties with respect to previous reforming catalyst.

### 5.3 Value-Chain

There are a very large number of petrochemicals produced from the BTX aromatics. The following diagram shows the chains leading from the BTX components to some of the petrochemicals that can be produced from those components, **Figure 7**.



**Figure 7 - The Chain of Petrochemicals Derived from The BTX Aromatics**

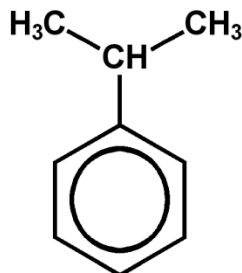
### 5.4 Marketing Data

- Global consumption of benzene, estimated at more than 40,000,000 tons in 2010
- Para-xylene consumption is growth by 10% from 2009 to 2010 with 2,800,000 tons.
- For the consumption of benzene in the United States, just under half of the benzene in the US is consumed in the production of EB for styrene.
- Toluene is primarily used as a component in gasoline, the blending value of toluene is around 10 percent higher than benzene's.

## 6. Cumene

### 6.1 Chemical Structure

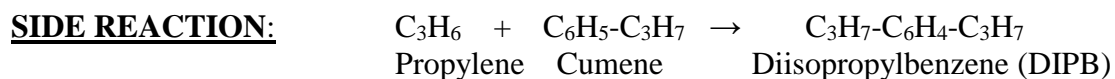
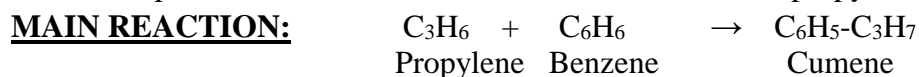
**Cumene** is the common name for **isopropyl benzene**, an organic compound that is based on an aromatic hydrocarbon with an aliphatic substitution.



Cumene Structure

### 6.2 Manufacturing Process

Cumene is produced from the reaction between benzene and propylene as follows:



See **Table 9** and **Figure 8** for more details about UOP process.

**Table 9 – BTX, UOP Production Process Data**

<b>Process Name</b>	Honeywell UOP Cumene Process	
<b>Process type</b>	Continuous	
<b>Feedstock</b>	Benzene and Propylene	
<b>Product</b>	Cumene (isopropyl benzene)	
<b>Side Products</b>	Diisopropylbenzene (DIPB)	
<b>Pressure</b>	25 atm	
<b>Temperature</b>	350°C	
<b>Catalyst</b>	<i>Old</i>	<i>Present (New)</i>
	<i>Solid phosphoric acid</i>	<i>Zeolites</i>
<b>Reaction phase</b>	Liquid and gas phases, but high conversion are obtained at gas phase reactions	
<b>Reaction type</b>	<b>Exothermic</b>	
<b>Reactor type</b>	Shell and tube reactors	

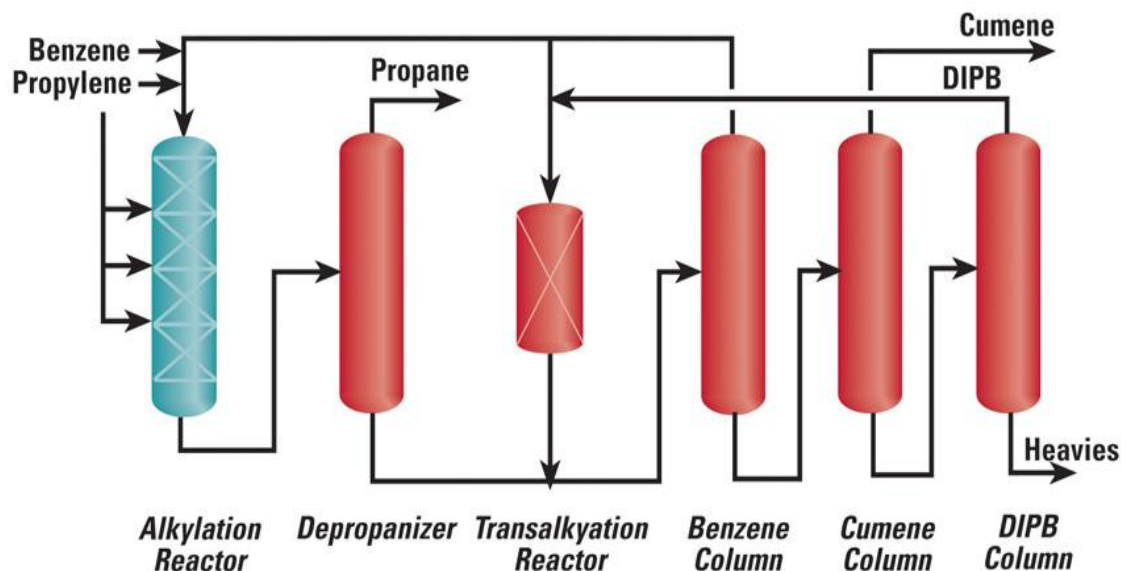
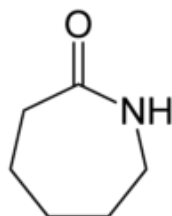


Figure 8 - The Chain of Petrochemicals Derived from The BTX Aromatics

## 7. Caprolactam

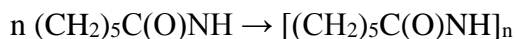
### 7.1 Chemical Structure

It is an organic compound with the formula  $(\text{CH}_2)_5\text{C}(\text{O})\text{NH}$  which is a lactam of 6-aminohexanoic acid (ε-aminohexanoic acid, aminocaproic acid). This colourless solid is a lactam or a cyclic amide of caproic acid. Approximately 2 billion kilograms are produced annually. It is the precursor to Nylon 6, a widely used synthetic polymer.



Caprolactam

Almost all caprolactam produced goes **into the production of Nylon-6**. The conversion entails a ring-opening polymerization:



Nylon-6 is widely used in fibers and plastics.

### 7.2 Manufacturing Process

Currently, practically all commercial caprolactam production globally is based on aromatics feedstock. However, over 95 percent of this global production is either from cyclohexane (from benzene) or phenol via cyclohexanone and the cyclohexanone oxime.

### 7.2.1 Caprolactam Aromatics Feedstock based Technologies

- i. DSM process
- ii. Honeywell phenol process
- iii. Cyclopol process
- iv. Toray photonitroization process
- v. EniChem ammoximation
- vi. Sumitomo rearrangement
- vii. SNIA Viscosa toluene process

Conventional caprolactam technology is based on the key intermediate cyclohexanone, which is usually produced by the oxidation of cyclohexane, but can also be made from phenol or toluene. Separately, hydroxylamine sulphate is manufactured by the oxidation of ammonia to nitrous oxide followed by hydrogenation in the presence of sulphuric acid. The hydroxylamine sulphate is then reacted with the cyclohexanone to produce cyclohexanone oxime. This is followed by a Beckmann rearrangement using oleum to yield caprolactam.

A disadvantage of existing technology is that large amounts of ammonium sulphate - up to 4.5 tonnes/tonne of caprolactam - are produced. Much development work is concentrating on reducing or even eliminating this byproduct. For example, DSM's HPO-plus process has substantially reduced this byproduct to 1.5 tonnes/tonne of caprolactam.

### 7.3 Market Data

- The nylon fibers market is at around 1%/year growth while demand for engineering resins is much stronger at 4-5%/year. Overall long-term global growth for caprolactam is estimated in the range of 2-2.5%/year.
- Global trade in caprolactam will decrease as Asia becomes more self-sufficient.
- China is expected to continue to be an importer of caprolactam. China is expected to be able to produce 660,000 tons/year but with demand estimated at 1.0-1.1m tons; imports of 400,000-500,000 tons will still be needed.

## 8. Nylon 6 (PA6)

### 8.1 Chemical Structures

**Nylon 6 (Polyamide)** or **polycaprolactam** is a polymer and nylon 6 is not a condensation polymer, but instead is formed by ring-opening polymerization.

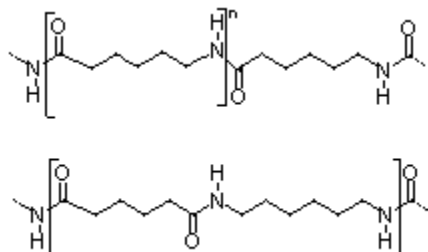
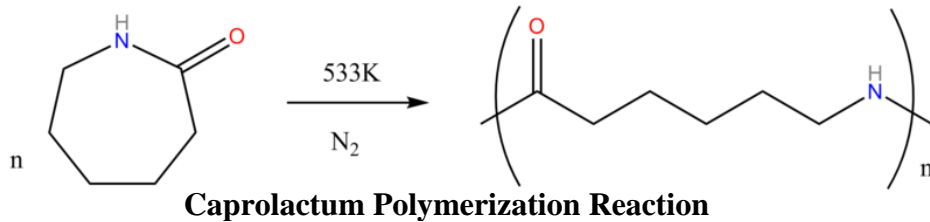


Figure 9 - Nylon 6 (upper) and Nylon 6,6 (lower)



## 8.2 Manufacturing Process

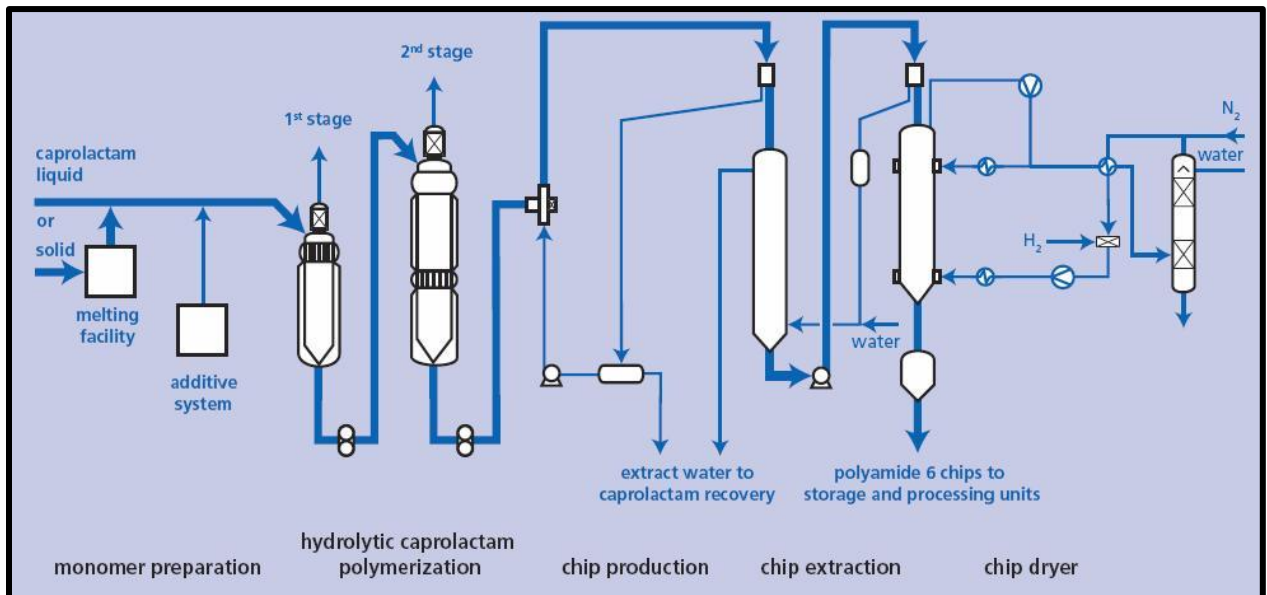
Nylon 6 begins as pure caprolactam. Caprolactam has 6 carbons. When caprolactam is heated at about 533 K in an inert atmosphere of nitrogen for about 4-5 hours, the ring breaks and undergoes polymerization. Then the molten mass is passed through spinnerets to form fibres of Nylon 6.



*Zimmer® Polyamide Technology; (Table 10, Figure 10)*

**Table 10 – Zimmer® Polyamide Technology Data**

<b>Technology Name</b>	Zimmer® polyamide technology
<b>Licenser</b>	Lurgi company
<b>Process type</b>	Continuous operation in two-stage
<b>Feedstock</b>	Caprolactam liquid or solid
<b>Product</b>	Polyamide 6 (Nylon 6)
<b>polymerization catalyst</b>	Titanium dioxide
<b>Production capacity</b>	300 t/day
<b>Operating condition</b>	Normal conditions
<b>Conversion</b>	90%



### 8.3 Applications

Typical application examples are:

- Gears and sprockets
- Hammer heads
- Impact and shock resistant components

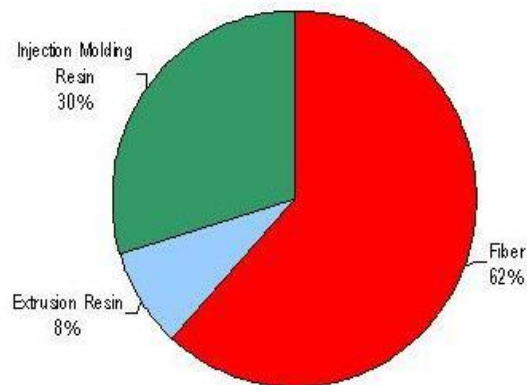
Typical applications of PA6 and PA66 are shown below in **Figure 11**



**Figure 11 - Typical applications of PA6 and PA66**

### 8.4 Market Data

- Currently the annual global consumption of PA6 and PA6.6 is about 6.8 million tons.
- PCI expects the global polyamide market to grow by 2.4 percent annually till 2020.
- Among most types of polyamide, approximately 85-90 percent of nylon in the global market are nylon 6 and nylon 6,6.
- Global nylon consumption by end-use is shown below in **Figure 12**.



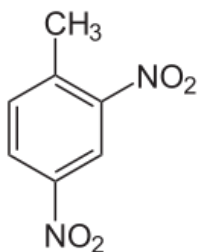
**Figure 12 - Global Nylon Consumption by End-Use**

- **World demand for Nylon 6**
  - ✓ Strong demand for nylon 6 in China is leading market growth for the engineering polymer, says Chemical Market Associates Inc (CMAI), which forecasts global demand to grow at an average annual rate of close to 5% up to 2015.
  - ✓ Asia has become the largest nylon 6 consuming region.
  - ✓ Global demand for nylon 66 engineering resin is forecast to grow at an average rate of close to 6% per year up to 2015.
  - ✓ Most of the growing demand for polyamides is needed to supply China which already consumes around 30% of the global polyamide production (38% of PA6 and 15% of PA66, respectively).

## 9. Di-Nitrotoluene (DNT)

### 9.1 Chemical Structure

**2, 4-Dinitrotoluene (DNT)** is an organic compound with the formula  $\text{CH}_3\text{C}_6\text{H}_3(\text{NO}_2)_2$ . This pale yellow crystalline solid is well known as a precursor to trinitrotoluene (TNT) but is mainly produced as a precursor to toluene diisocyanate (TDI).



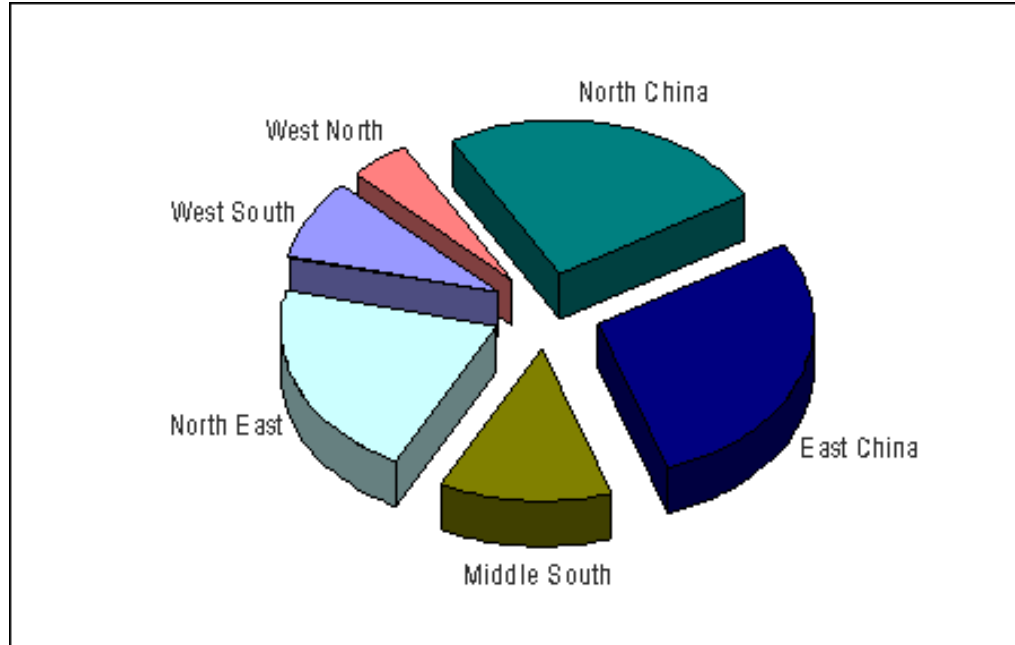
**DNT Structure**

### 9.2 Applications

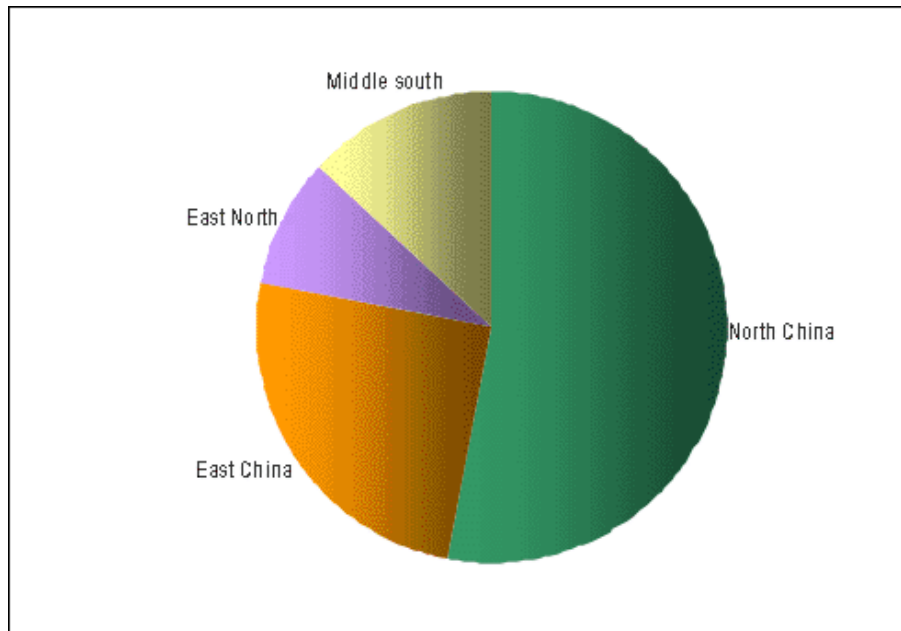
- The predominant use of 2,4-dinitrotoluene is as an intermediate in the manufacture of polyurethanes.
- 2,4-Dinitrotoluene is also used for the production of explosives, for which it is a gelatinizing and waterproofing agent.
- Other applications include uses as an intermediate in dye processes and in smokeless gunpowders.

### 9.3 Market Data

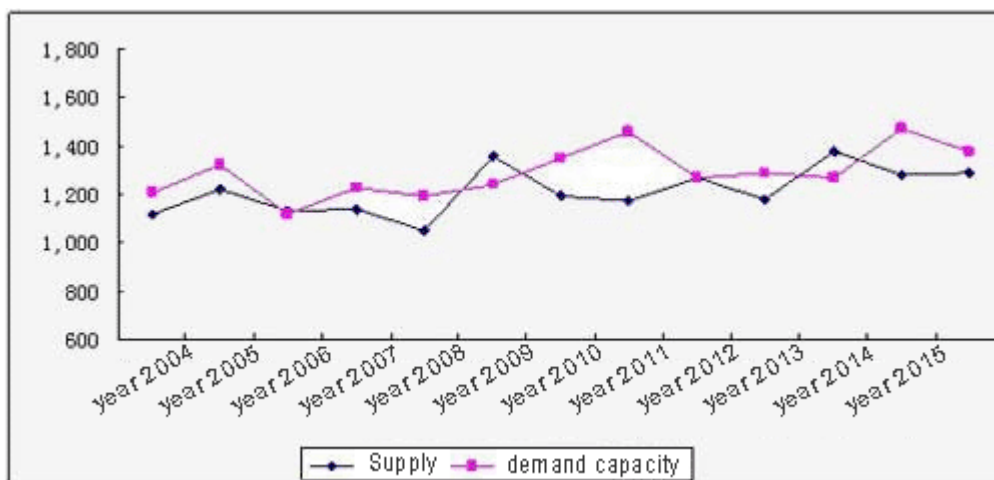
Analysis of Region Distribution for DNT about Demand illustrated in **Figure 13**, where DNT structure analysis of producing region is shown in **Figure 14**, also Analysis of Supply-Demand DNT Balance for china has been studied in **Figure 15**.



**Figure 13 - Analysis of DNT Region Distribution about Demand**



**Figure 14 - Structure Analysis of DNT Producing Region**

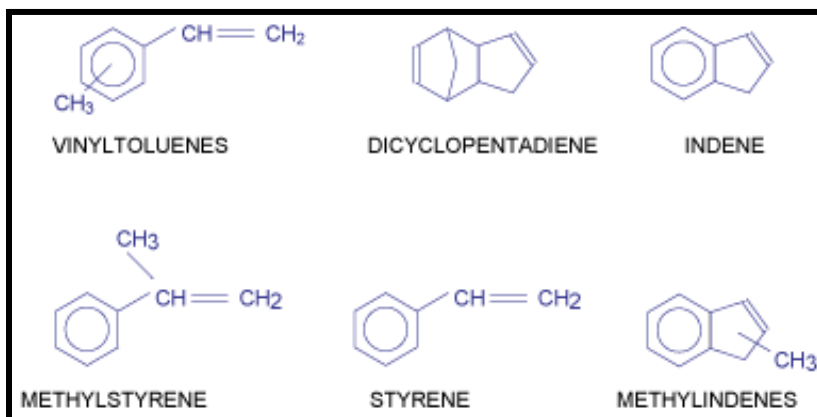


**Figure 15 - Analysis of DNT Supply-Demand Balance**

## 10.C9 Resins

### 10.1 Chemical Structure

As discussed in the C5 section, Aliphatic Resins, the feedstocks for hydrocarbon resins are produced via cracking of naphtha. Basic C9, aromatic resins are produced from C9 resin oil that contains various monomers as illustrated in **Figure 16**.



**Figure 16 - C9 Resin Oil Composition**

C9 Hydrocarbon Resin is a kind of Aromatic Hydrocarbon resin produced by C9 fraction, by products of petroleum cracking, through pretreatment, polymerization and distillation. It isn't a high polymer but a low polymer with the molecular weight between 300-3000.

## 10.2 Applications

- **Paints**

Paints mainly use C9 Hydrocarbon Resin with high softening points, C9 Hydrocarbon Resin added to paints can increase the final finishes of paints, the adhesiveness of paint films and the hardness. Resistance to acid and alkaline.

- **Rubbers**

Mainly use C9 Hydrocarbon Resin with low softening points, the resin has very good mutual solubilities with natural rubber particles, No effect to the sulphurization of rubber.

- **Adhesives**

The resins have very good adhesiveness; they can increase the adhesiveness of adhesives, resistance to acid, alkaline and water. Subsequently they will reduce the production cost.

- **Printing inks**

Usually, C9 Hydrocarbon Resin which have high softening point are used for printing inks, they have color spreading, fast dry and brightening effects and will increase the printing property.

- **Others**

C9 Hydrocarbon Resin has certain unsaturation property and can be used as paper glutting agents, plastic modifiers etc.

## 11. Conclusion

The market demand and the economic analyses of each chemical should be considered strictly due to the fact that the prices of different chemicals depend on the demand in each country. Understanding the several process technologies will allow us to select the best option that is relevant to a specific country as well as saving money and producing at the same time. It is possible to estimate the future demand or supply just by looking at the market data of the different chemicals that we have discussed.

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