Nature of Invention: Chemical molecule and synthesis route

Applicant: ChemiEvolve Industries Limited

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Chemical Formula: $(C_6H_6O \cdot CH_2O)_n$

Chemical Name: Polyoxybenzylmethyleneglycolanhydride(Phenol-Formaldehyde Resin)

CAS Number – 9003-35-4

Chemical Synthesis Route

- **Lab Scale Method:-**

Raw Materials: - Phenol ,Formaldehyde,Ammonia(Basic Solution)

Formaldehyde: -

Formaldehyde is produced industrially by the catalytic oxidation of methanol. The most common catalysts are silver metal, iron molybdenum oxides with a molybdenum -enriched surface, or Vanadium oxides. In the commonly used formox, methanol and oxygen react at c. 250–400 °C in presence of iron oxide in combination with molybdenum and/or vanadium to produce formaldehyde according to the chemical reaction:
$2\ CH_3OH + O_2 \rightarrow 2\ CH_2O + 2\ H_2O$

The silver-based catalyst usually operates at a higher temperature, about 650 °C. Two chemical reactions on it simultaneously produce formaldehyde: that shown above and the dehydrogenation reaction:
$CH_3OH \rightarrow CH_2O + H_2$

In principle, formaldehyde could be generated by oxidation of methane, but this route is not industrially viable because the methanol is more easily oxidized than methane.

Phenol:-

Generally Phenol is prepared from the process known Cumene Process,

It involves the partial oxidation of cumene (isopropyl benzene) via the Hock Rearrangement.

The synthesis of Bakelite involves the reaction between phenol and formaldehyde under heat and pressure. This reaction is known as condensation polymerization. Here's a simplified equation representing the reaction:
Phenol + Formaldehyde → Bakelite + Water

It begins with the heating of phenol and formaldehyde in the presence of a catalyst such as hydrochloric acid, zinc chloride, or the base ammonia. This creates a liquid condensation product, referred to as *Bakelite A*, which is soluble in alcohol, acetone, or additional phenol. Heated further, the product becomes partially soluble and can still be softened by heat.

Sustained heating results in an "insoluble hard gum". However, the high temperatures required to create this tend to cause violent foaming of the mixture when done at standard atmospheric pressure, which results in the cooled material being porous and breakable.
The polymerization process makes the layers hard, rigid, and dense. The operating temperature of Bakelite ranges from 160 °F (70 °C) for nylon reinforced Bakelite, which has superior electrical properties in humid conditions, to 250 °F (120 °C) for canvas-reinforced Bakelite.
The process described herein involves the gradual addition of aqueous formaldehyde, containing 35-60 percent by weight of formaldehyde, to a phenol maintained at a temperature of 60°-100° C., preferably 70°-90° C., and at a reduced pressure of 11-26 inches of mercury in the presence of an alkaline catalyst. The rate of formaldehyde addition is such that the exothermic reaction aids in maintaining the stated temperature range and thereby simultaneously distils approximately all the water added with the formaldehyde and that formed by the condensation so that the volume of the reaction mass is maintained approximately constant. This constant volume allows efficient use of the equipment.

Lower temperatures might result in a more linear structure (Novolac resin), while higher temperatures promote extensive cross-linking, leading to a more rigid Bakelite. These are obtained by the condensation reaction of phenol with formaldehyde in the presence of either an acid or a base catalyst. The reaction starts with the initial formation of o- and/or p-hydroxymethylphenol derivatives, which further react with phenol to form compounds having rings joined to each other through–CH2 groups. The initial product could be a linear product – Novolac used in paints.

Novolac on heating with formaldehyde undergoes cross linking to form an infusible solid mass called bakelite. It is thermosetting polymer which cannot be reused or remoulded. Thus, bakelite is formed by cross linking of linear chains of the polymer novolac.
The process consists of three phases.

- The product from the first phase, called the initial condensation product, is designated Bakelite A. At ordinary temperatures, Bakelite A may be liquid, viscous, pasty, or solid and is soluble in alcohol, acetone, phenol, and NaOH solution.
- The product from the second phase, the intermediate condensation product, is designated Bakelite B. It is solid at all temperatures and is insoluble in all solvents but may swell in acetone, phenol, or terpineol. It softens during heating and becomes elastic but does not melt and becomes hard and brittle upon cooling.
- The product from the third phase is called the final condensation product, or Bakelite C. It is infusible, insoluble in all solvents, and indifferent to ordinary acids and alkaline solutions. Other properties of Bakelite C include poor conductivity of heat and electricity and excellent thermal stability.

Bakelite is the trademark of oxybenzylmethylen-glycolanhydride.

Thermodynamic Favorability:

The formation of Bakelite is a **condensation reaction**, where a small molecule (water) is eliminated as the larger Bakelite molecule forms. This removal of water molecules increases the system's entropy (disorder), making the reaction thermodynamically favorable ($\Delta G < 0$).

- **Molar ratio of Phenol to Formaldehyde:** This ratio influences the final Bakelite structure. A higher phenol content might require slightly higher temperatures to achieve a desirable reaction rate due to the increased steric hindrance (bulkiness) of the molecule.

- Yield: The yield of bakelite synthesis can vary, but it's typically high under optimised conditions. Condensation polymerization reactions like the one involved in bakelite formation generally proceed at high conversion rates. However, some factors, such as incomplete reactions, side reactions, or loss during purification processes, can affect the yield. Generally, yields of upwards of 90% are achievable with efficient synthesis methods.
- Purity: The purity of bakelite refers to the absence of impurities and the degree to which the desired polymer is formed. High-purity bakelite is desirable for ensuring its mechanical, electrical, and thermal properties meet the intended application requirements. Impurities can arise from incomplete reactions, contamination of raw materials, or side reactions. Purity can be assessed through analytical techniques such as spectroscopy, chromatography, and elemental analysis. Typically, the purity of Bakelite is very high, often exceeding 99%.

It was named a National Historic Chemical Landmark by the American Chemical Society.

APPLICATION AREAS:

High heat-resistant up to 285°C, Baking oven rollers, cookware fittings.

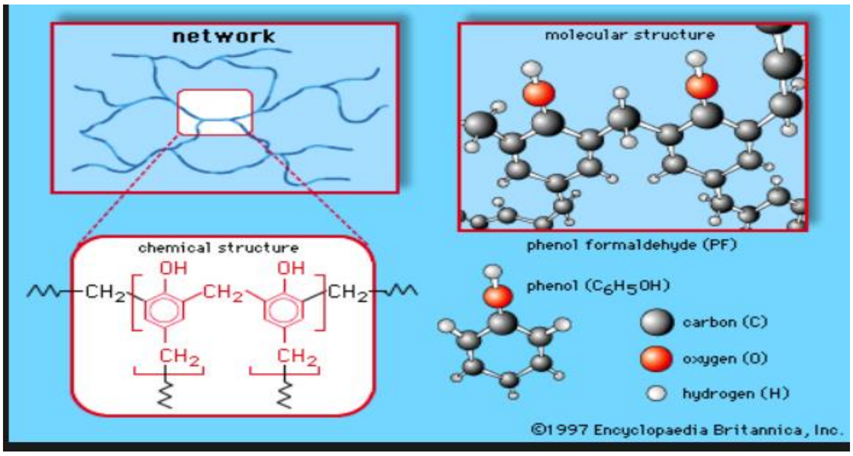
Lab Research R&D :-

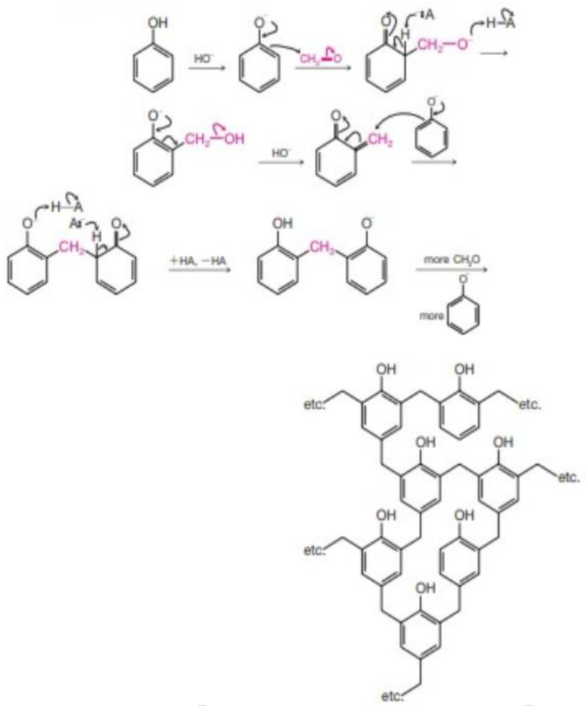
We are working on our materials to achieve at low cost and optimizing conditions using Genetic Algorithm where several parameters are being taking into account in low cost economics.

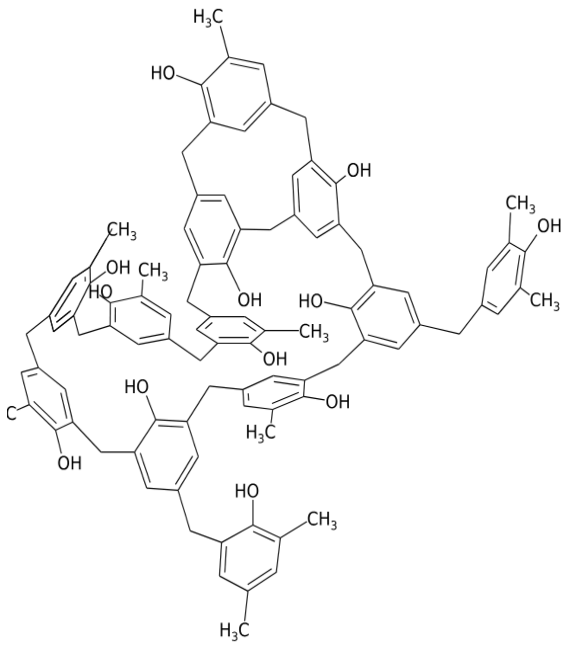
Also In our Lab,

We are researching about CO2 capture from Porous Bakelite polymer to reduce release of CO2 into Atmosphere while burning fossil fuels .

From Thermodynamically ,Kinetically View using DFT simulation in our approach .







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Bakelite® First Synthetic Plastic - National Historic Chemical Landmark - American Chemical Society (acs.org)

▷ Bakelite process | Chemistry Online (chemistry-online.com)

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https://en.wikipedia.org/wiki/Bakelite#cite_note-Landmark-5

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