Nature of Invention: Chemical molecule and synthesis route

Applicant: SynthoChem

Inventors: Keerthi S

Chemical Formula: $C_7H_6O_3$

Chemical Name: Salicylic Acid

Chemical synthesis routes: Kolbe-Schmitt

a. How can you prepare this chemical at lab-scale? List raw materials and chemicals needed. List reaction steps (product yield) and separation steps (final purity). If possible, give reaction conditions.

Salicylic acid can be synthesized in the lab by the Kolbe-Schmitt reaction, which involves the reaction of phenol (C6H5OH) with sodium hydroxide (NaOH) and carbon dioxide (CO2). The reaction proceeds as follows:

Step 1: Phenol reacts with sodium hydroxide to form sodium phenoxide.

C6H5OH + NaOH → C6H5ONa + H2O

Step 2: Sodium phenoxide reacts with carbon dioxide to form salicylic acid.

C6H5ONa + CO2 → C6H4(OH)CO2Na C6H4(OH)CO2Na + HCl → C6H4(OH)CO2H + NaCl

The raw materials and chemicals needed for the synthesis of salicylic acid are:

- Phenol
- Sodium hydroxide
- Carbon dioxide
- Hydrochloric acid (HCl)
- Water
- Ice
- Ethanol

The reaction conditions are as follows:

- Temperature: Room temperature (25°C)
- Pressure: Atmospheric pressure
- Time: 2-3 hours

The reaction yield depends on the purity of the raw materials and the reaction conditions. Typically, a yield of 70-80% can be achieved.

Separation steps:

1. After the reaction, the mixture is cooled to room temperature, and excess sodium hydroxide is neutralized with hydrochloric acid.
2. The resulting mixture is then extracted with diethyl ether to remove impurities.
3. The aqueous layer is then acidified with hydrochloric acid to precipitate salicylic acid.
4. The precipitated salicylic acid is filtered, washed with water, and dried under vacuum to obtain the final product.

The purity of the salicylic acid can be checked by measuring its melting point, which should be around 158-161°C for pure salicylic acid.

b. Are there any alternative synthesis routes to prepare this compound? List raw materials and chemicals needed. List reaction steps (product yield) and separation steps (final purity). If possible, give reaction conditions.

Yes, there are alternative synthesis routes to prepare salicylic acid. One such method is the hydrolysis of methyl salicylate with a strong base such as sodium hydroxide. The reaction proceeds as follows:

Methyl salicylate + NaOH → Salicylic acid + Methanol + NaOH

The raw materials and chemicals needed for this synthesis are:

- Methyl salicylate
- Sodium hydroxide
- Water
- Ethanol

The reaction conditions are as follows:

- Temperature: 60-70°C
- Pressure: Atmospheric pressure
- Time: 2-3 hours

The reaction yield depends on the purity of the raw materials and the reaction conditions. Typically, a yield of 90-95% can be achieved.

Separation steps:

1. After the reaction, the mixture is cooled to room temperature, and excess sodium hydroxide is neutralized with hydrochloric acid.
2. The resulting mixture is then extracted with diethyl ether to remove impurities.

3. The aqueous layer is then acidified with hydrochloric acid to precipitate salicylic acid.
4. The precipitated salicylic acid is filtered, washed with water, and dried under vacuum to obtain the final product.

The purity of the salicylic acid can be checked by measuring its melting point, which should be around 158-161°C for pure salicylic acid.

Another alternative method for the synthesis of salicylic acid is the oxidation of phenol using nitric acid. However, this method is less commonly used due to the high cost and hazards associated with nitric acid.

Overall, the hydrolysis of methyl salicylate is a more efficient and commonly used method for the synthesis of salicylic acid.

References: Provide reference for a research paper or an actual patent.

https://patents.google.com/patent/US3331750A/en

List the contributions of each author:

Keerthi S carried out the entire R&D of salicylic acid which included chemical finding, synthesis of the compound, separation steps, yield and percent purity estimation.

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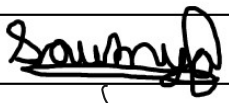
Name	Roll No	Signature
Saumya Gupta (CEO)	210944	
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