Nature of Invention: Chemical molecule and synthesis route

Applicant: QuantiVEX

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Chemical Formula: **($R\text{-}C_6H_4\text{-}SO_3Na$)**

Chemical Name: Linear alkyl benzene sulphonate

Chemical synthesis routes:

a. **Sulfonation of linear alkyl benzene**

Raw materials

1.Linear alkyl benzene($R\text{-}C_6H_4$)

2.SO_3 (sulphonating agent)

3. Hydrogen peroxide (a protic reagent and oxidising agent)

4. A Neutralizing agent

Sulfonation:

Reaction:

linear alkyl benzene + So_3(sulfonating agent) → linear alkyl benzene sulfonic acid

Mechanism:

Sulfonation of linear alkyl benzene (LAB) is an **electrophilic aromatic substitution (EAS)** reaction. The sulfonating agent, sulfur trioxide (SO_3), acts as an electrophile and attaches to the benzene ring of LAB.

1. **Activation of Sulfur Trioxide (SO_3):**
   a. SO_3 is a strong electrophile and reacts with benzene directly.
   b. It forms a highly reactive intermediate due to the resonance stabilization of the benzene ring.
2. **Formation of the Arenium Ion (σ-complex):**
   a. The benzene ring donates electrons to SO_3, forming an unstable carbocation (arenium ion).
   b. This intermediate is stabilized via resonance.
3. **Proton Transfer and Formation of the Product:**
   a. A base (often water or trace H_2SO_4) removes a proton from the arenium ion.
   b. This restores aromaticity, leading to the formation of **linear alkyl benzene sulfonic acid**.

Reaction Conditions:

- **Temperature:** 0 - 90°C (typically controlled to prevent over-sulfonation)
- **Solvent:** Can be carried out in a gas phase or liquid phase; sulfuric acid may be used as a solvent.

- **Reaction Type:** Highly **exothermic**, requiring efficient cooling.

Sulfonation Process: Detailed Mechanism and Kinetics

The **sulfonation of Linear Alkyl Benzene (LAB) follows first-order kinetics**, with the reaction rate expressed as:

$$r = k[LAB][H_2SO_4]^2[H_2O]^{-1}$$

where excess sulfuric acid increases reaction speed, but excess water formation slows it down. The activation energy for the reaction is **18.75 kcal/mol**, as determined from Arrhenius modeling .

To ensure complete conversion (>98%), the molar ratio of **LAB:H_2SO_4 should be maintained at 1:5**. The **semi-batch reactor configuration** with **controlled acid addition** helps manage exothermic heat release. A **cooling jacket** is required to maintain **optimal reaction temperature (60°C)**.

Bleaching:

Reaction:

linear alkyl benzene sulfonic acid + hydrogen peroxide →linear alkyl benzene sulfonic acid

(Dark coloured) (Light coloured)

Mechanism:

1. Oxidation of Impurities:
    a. Impurities (e.g., polymeric species, oxidized byproducts) contain conjugated double bonds, leading to colour.
    b. H_2O_2 oxidizes these compounds, breaking their extended conjugation and rendering them colourless.
2. Radical Formation:
    a. Under suitable conditions, H_2O_2 decomposes to form hydroxyl radicals (·OH).
    b. These radicals oxidize organic impurities to CO_2 and water.

Reaction Conditions:

- Temperature: 0 - 50°C
  - Higher temperatures accelerate oxidation but may degrade the product.
- Catalyst: Sometimes metal catalysts (e.g., sodium tungstate) are used to enhance bleaching efficiency.
- Solvent: The reaction is typically carried out in an aqueous medium.

Neutralization:

Reaction:

Linear alkyl benzene sulfonic acid $\xrightarrow[\text{(Neutralizing agent)}]{}$ linear alkyl benzene sulfonate

_Mechanism:

1. **Acid-Base Reaction:**
   a. The sulfonic acid ($-SO_3H$) group reacts with a base, donating a proton (H^+).
   b. This forms the corresponding **sulfonate salt ($-SO_3^- Na^+$)**.
2. **Salt Formation and Stabilization:**
   a. The product (linear alkyl benzene sulfonate, or **LAS**) is **water-soluble** and **stable**.
   b. This reaction prevents further oxidation and degradation.

Reaction Conditions:

- **Temperature:** Room temperature to 50°C
- **pH control:** The final solution must be **mildly alkaline (pH ~7-8)** to ensure complete neutralization.
- **Agitation:** Stirring is essential to ensure uniform mixing.

Purity Testing and Final Product Evaluation

After synthesis, the **quality of LAS** is determined using:

1. **FTIR/NMR spectroscopy**: Confirms sulfonate ($-SO_3^-$) formation.
2. **Titration of residual acid**: Ensures neutralization is complete.
3. **High-Performance Liquid Chromatography (HPLC)**: Detects byproducts to maintain commercial-grade purity.

Scaling Up: Industrial Considerations

For **large-scale production**, Falling Film Reactors (FFR) are used to improve **reaction efficiency and heat management**. The **final product is spray-dried** to produce LAS in **powdered form**, making it ideal for detergent formulations.

References:

1)https://patents.google.com/patent/US2827484A/en

2)https://pmc.ncbi.nlm.nih.gov/articles/PMC8867685/

3)https://hithaldia.in/eccn/vol6_1a/J5_6.pdf

4)https://patentimages.storage.googleapis.com/1b/67/78/712514f5f0fc50/WO1997014676A1.pdf

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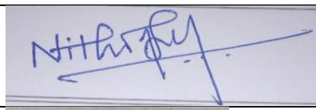
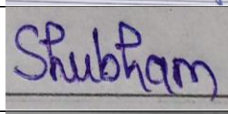
CEO Name	Nithin TM	
First author Name	Shubham Singh	
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