Nature of Invention: Chemical molecule and synthesis route

Applicant: ChemEverse

Inventors: Manas Todi

Chemical Formula: $C_{12}H_{25}(OCH_2CH_2)_2OSO_3Na$

Chemical Name: Sodium Laureth-2 Sulfate

Chemical synthesis routes:

a) LAB SCALE SYNTHESIS:

1) SO_3 Sulfation Process: [1]

<u>Raw Materials and Chemicals</u>:

1) Dodecyl alcohol/Lauryl alcohol **($C_{12}H_{26}O$)** or fatty alcohol ethoxylate **($C_{12}H_{25}(OCH_2CH_2)_nOH$)**
2) Ethylene oxide **(C_2H_4O)**
3) Sulfur trioxide **(SO_3)** or Chlorosulfonic acid **(HSO_3Cl)**
4) Sodium hydroxide solution **(NaOH, ~50 wt%)**

<u>Reaction Steps</u>:

Step 1 : Ethoxylation

$$\underset{\text{(Dodecyl Alcohol)}}{C_{12}H_{25}OH} + n\ \underset{\text{(Ethylene Oxide)}}{C_2H_4O} \rightarrow \underset{\text{(Lauryl Alcohol Ethoxylate)}}{C_{12}H_{25}(OCH_2CH_2)_nOH}$$

Conditions:[2]

a) Temperature: Typically 150–180°C
b) Pressure: Elevated pressure (~2–5 bar)
c) Catalyst: Alkaline catalyst (e.g., KOH)

Yield: High yield (>90%)

Step 2 : Sulfation

$$\underset{\text{(Lauryl Alcohol Ethoxylate)}}{C_{12}H_{25}(OCH_2CH_2)_nOH} + \underset{\text{(Sulfur trioxide)}}{SO_3} \rightarrow \underset{\text{(Lauryl Ether Sulfate (Acid form))}}{C_{12}H_{25}(OCH_2CH_2)_nOSO_3H}$$

Conditions:[3]

1) Temperature: Controlled at 25–30°C

2) Reactor type: Glass-lined stirred, jacketed reactor
3) Reaction time: ~2.5 hours under vacuum

Yield: Generally high (>95% conversion)

Step 3: Neutralization

$$\underset{\text{(Lauryl Ether Sulfate (Acid form))}}{C_{12}H_{25}(OCH_2CH_2)_nOSO_3H} + NaOH \rightarrow \underset{\text{(Sodium Laureth-2 Sulfate)}}{C_{12}H_{25}(OCH_2CH_2)_nOSO_3Na} + H_2O$$

Conditions:[3]

1) Temperature: Below 45°C
2) Neutralizing agent: Sodium hydroxide solution (~50 wt%)

Yield: High yield, typically resulting in ~70 wt% active SLES solution

Separation and Purification Steps:

1. Scrubbing: Gaseous by-product HCl or SO_3 vapors are scrubbed using process water to produce dilute hydrochloric acid (~33 wt%) as a by-product.
2. Packing and Storage: Final SLES solution (~70 wt% active matter) is packed into drums for storage and distribution.

Final Purity: Typically, the final product purity is around 70 wt% active SLES, suitable for personal care and cleaning applications.

b) Alternative Processes:

1) Ziegler-Alfol Process:[1]

Raw Materials and Chemicals:

1) (Ethylene) (C_2H_4)
2) Aluminum metal
3) Hydrogen gas (H_2)

Reaction Steps:

Step 1: Formation of Triethylaluminum

$$\underset{\text{(Ethylene)}}{6\,C_2H_4} + 2\,Al + 3\,H_2 \rightarrow \underset{\text{(Triethylaluminum)}}{2\,Al(C_2H_5)_3}$$

Step 2: Chain Growth (Oligomerization)

$$\underset{\text{Triethylaluminium}}{Al(C_2H_5)_3} + n\ \underset{\text{ethylene}}{C_2H_4} \rightarrow \underset{\text{trialkylaluminum}}{Al(C_{2n+2}H_{4n+5})_3}$$

Conditions:[4]

1) Temperature: 60–120°C
2) Pressure: Elevated (~100 bar)
3) Catalyst: Triethylaluminum catalyst

Step 3: Oxidation to Fatty Alcohol

$$\underset{\text{Trialkylaluminum}}{Al(C_{2n+2}H_{4n+5})_3} + \underset{\text{air/oxygen}}{O_2/H_2O} \rightarrow \text{Fatty Alcohol} + Al(OH)_3$$

Temperature: 60–120°C [5]

Yield: Typically high (>85%) for fatty alcohol production; explicit numeric yields depend on reaction conditions but generally high in industrial practice.

Separation Steps:

1) Fatty alcohols separated via distillation columns.
2) Purity typically >95% linear primary fatty alcohols.

Note: To produce SLES from these fatty alcohols, subsequent ethoxylation and sulfation steps described previously must be performed.

2) OXO Process (Hydroformylation Route):[1]

Raw Materials and Chemicals Needed:

1) Olefins (e.g., C_{11} alkenes derived from petrochemical sources)
2) Carbon monoxide (CO)
3) Hydrogen gas (H_2)
4) Catalyst: Transition metals like cobalt or rhodium complexes

Reaction Steps:

Step 1: Hydroformylation

$$\text{Olefin} + \text{CO} + \text{H}_2 \longrightarrow \text{Aldehyde}$$

Conditions:

1) Temperature: ~90–150°C

2) Pressure: High pressure (~50–200 bar)
3) Catalyst: Cobalt or rhodium complexes

Yield: typically >90% aldehyde formation under optimized conditions.

Step 2: Hydrogenation of Aldehydes

$$\text{Aldehyde} + H_2 \rightarrow \text{Fatty Alcohol}$$

Temperature ~100–200°C; Pressure ~20–30 bar.

Yield: typically >95%.

Note: To produce SLES from these fatty alcohols, subsequent ethoxylation and sulfation steps described previously must be performed.

Method	Advantages	Disadvantages	Ideal Use
Ethoxylation & Sulfation	High purity, flexible scale	May require more specialized equipment	Personal care products
Ziegler Process	Selective product, consistent quality	Requires specific catalysts	Eco-friendly and sustainable products
OXO Process	High throughput, versatile feedstocks	Possible impurities in the final product	Industrial applications with cost concerns

References:

1) https://www.chemger.com/how-to-make-sles-liquid/
2) https://patents.google.com/patent/CN102276428A/en
3) https://cdn.intratec.us/docs/reports/previews/sles-e11a-b.pdf
4) https://patents.google.com/patent/US2781410A/en
5) http://en.shbinjia.cn/news/23.html

List the contributions of each author:

Manas Todi

1. Conducted a review of existing synthesis methodologies for SLES, including LAB-scale sulfation, Ziegler-Alfol process, and OXO process.
2. Collected and analyzed reference materials including patents and reports.
3. Researched and compiled optimal reaction conditions
4. Compared different synthesis methods in terms of efficiency, scalability, and industrial applicability based on published data.
5. Systematically documented reaction steps, conditions, and separation techniques.
6. Authored and structured the technical documentation for the invention, ensuring all chemical processes were clearly described and well-referenced.

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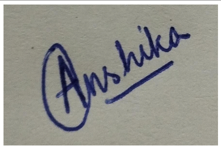
Anshika Agrawal	230160	
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