

Applicant: National Chemicals Limited (NCL)

CEO: Sidhant Thalor (221055)

Report Authors: 1. Tasneet Singh (221136)
2. Komal Kumari (220540)
3. Abhay Pratap Singh (220025)

Chemical Formula: $C_{13}H_{19}Br_2ClN_2O$

Chemical Name: trans-4-(2-Amino-3,5-dibromobenzylamino)-cyclohexanol

Common Name: Ambroxol Hydrochloride (Ambroxol)

Use case:

a. What is the use of this compound?

Ambroxol is a clinically validated mucolytic agent (breaks down and thins the mucus, making coughing easier). It is used to clear congestion in respiratory diseases. Ambroxol is also used as a pain reliever for sore throats as it has a local numbing effect. It also has Anti-inflammatory and Antioxidant properties. It is used in treatment of Tracheobronchitis, Pneumoconiosis, Chronic inflammatory pulmonary conditions, Bronchiectasis, Asthma and many more unmentioned diseases whose new cases are increasing with each year passing.

b. Are there any alternatives to this compound? Name a few.

Some alternatives to Ambroxol include:

- Dextromethorphan (DM)
- Guaifenesin
- Codeine
- Bromhexine

Each of these alternatives exhibits unique characteristics and mechanisms of action.

c. Why is this compound superior to its alternatives?

Dextromethorphan (DM), for instance, primarily targets the brain's cough centre, thereby reducing the urge to cough. However, it does not address the underlying cause of the cough.

Guaifenesin, on the other hand, is limited by its lack of anti-inflammatory properties. This property is essential for the treatment of pneumonia.

Codeine, a derivative of Morphine, is found in some cough syrups. However,

due to its narcotic property there is a risk of addiction and misuse associated with it. Bromhexine, while effective, lacks additional therapeutic properties and safety profile.

d. Is this compound imported in India? What is the magnitude of imports?

Yes, Ambroxol is imported into India. As per Zaubas's India Import data, \$103,520 worth of Ambroxol was imported in India. But this is nothing in front of what was exported by India. As per the same source \$26,491,725 worth of Ambroxol was exported by India to 100+ different countries. The main markets of Ambroxol are Mexico, Russia, Indonesia, Brazil and Germany. The global market has high demand for Ambroxol with fewer competitors and is growing with a CAGR of 5.2%.

Economic feasibility:

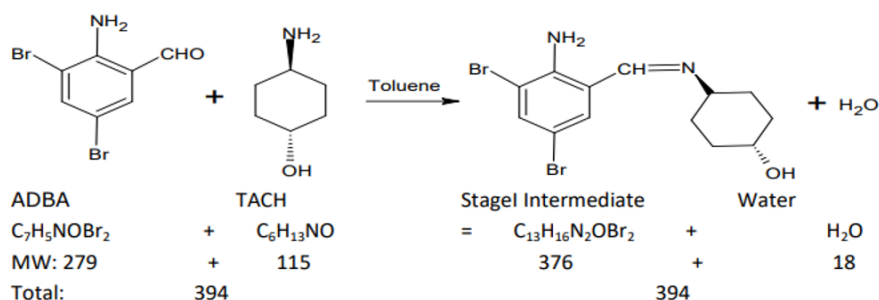
a. What input raw materials are needed for its synthesis (same as reported in the Patent application)?

SNo.	Raw Material	Cost (Rs)	Molecular Mass
1.	2-Amino-3,5-Dibromobenzaldehyde (C ₇ H ₅ NOBr ₂)	1400 Rs/kg	279 kg/kmol
2.	Trans-4-aminocyclohexanol (C ₆ H ₁₃ NO)	2000 Rs/kg	115 kg/kmol
3.	Hydrochloric Acid 38% solution (HCl)	10 Rs/kg	36.5 kg/kmol
4.	Sodium Borohydride (NaBH ₄)	2250 Rs/kg	38 kg/kmol
5.	Toluene (C ₆ H ₅ CH ₃)	156 Rs/kg	92.14 kg/kmol
6.	Methanol (CH ₃ OH)	36.1 Rs/kg	32kg/kmol
7.	Charcoal	8 Rs/kg	N.a

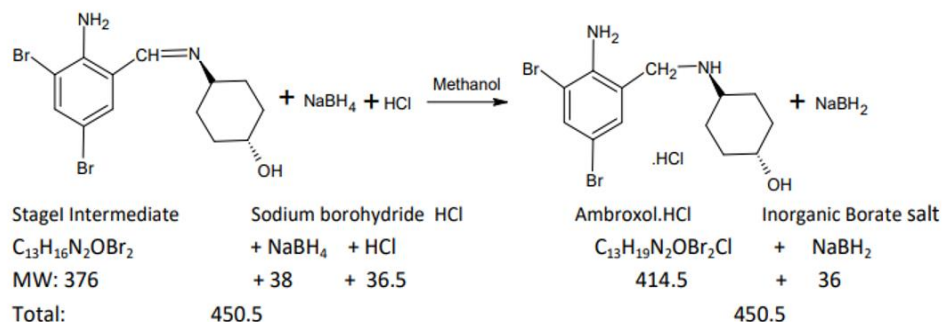
b. Provide preliminary economic feasibility based on cost of raw materials, solvents and product selling price.

Selling Price of Ambroxol	3000 Rs/kg
Molecular Mass of Ambroxol	414.56 kg/kmol

Economic feasibility: For production of 1000 kg of Ambroxol.



Stage 1 reaction efficiency - 90%



Stage 2 reaction efficiency - 70%

Raw material Cost:

$$= 2.41/0.7 \times (36.5 \times 30 + 38 \times 2250/2 + 36.5 \times 560/2) + 3.82 \times (279 \times 1400 + 115 \times 2000) = 2,564,559 \text{ Rs per 1000 kg of Ambroxol}$$

Profitability:

$$3,000,000 - 2,564,559 = 435,440 \text{ Rs per 1000 kg of Ambroxol produced.}$$

*Assuming $NaBH_2$ is regenerated to $NaBH_4$ with 50% efficiency.
Toluene and Methanol. are catalysts and hence fully recovered.

References:

- Uses: [link1](#), [link2](#), [link3](#).
- Alternatives and differentiator : [link](#).
- Imported data and CAGR: [link1](#), [link2](#).

- Cost of raw material used: [TACH](#), [ABDA](#), [NaBH₄](#), [ambroxol SP](#), [HCl](#), [toluene](#), [methanol](#).

List the contributions of each author:

- Tasneet was responsible for the research of uses, alternatives and differentiators of ambroxol.
- Tasneet and Komal carried out research to find the cost of raw material.
- Abhay and Komal did the research for the market size and demand of ambroxol globally as well as nationally. He calculated the economic feasibility and profitability.

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Applicant: National Chemicals Limited [NCL]

CEO: Sidhant Thalor (221055)

Report Authors: Khushi Aggrawal (220529)

Harsh Nirmal (220431)

Anushri Bhargava (220189)

Chemical Formula: C₅H₈O₂

Chemical Name: Acetylacetone

Use case:

a. What is the use of this compound?

Acetylacetone is primarily used as a versatile chemical intermediate in industries such as pharmaceuticals, agrochemicals, fragrances, and specialty chemicals. It serves as a key building block in organic synthesis, metal chelation processes, and as a solvent. Additionally, it is utilized in the production of pharmaceutical intermediates and fragrance compounds.

b. Are there any alternatives to this compound? Name a few.

Some alternatives to acetylacetone include benzoylacetone, dibenzoylmethane, EDTA, DTPA, and TTHA for specific applications such as organic synthesis, metal chelation, and solvents. These alternatives are chosen based on factors like reactivity, stability, and cost-effectiveness.

c. Why this compound is superior to its alternatives?

Acetylacetone's superiority over alternatives lies in its versatility in organic synthesis, strong metal chelation properties, moderate solubility and reactivity, widespread availability, cost-effectiveness, and compatibility with existing processes.

d. Is this compound imported in India? What is the magnitude of imports?

Yes, acetylacetone is imported into India. As per Volza's India Import data, Acetylacetone import shipments in India stood at 3.1K, imported by 121 India Importers from 120 Suppliers.

India imports most of its Acetylacetone from United States, Germany and China and is the largest importer of Acetylacetone in the World.

The top 3 importers of Acetylacetone are India with 3,126 shipments followed by Brazil with 545 and United States at the 3rd spot with 512 shipments.

Economic feasibility:

a. What input raw materials are needed for its synthesis (same as reported in the Patent application)?

1) Acetone: Acetone serves as one of the starting materials in the synthesis of acetylacetone. It undergoes a Claisen condensation reaction with acetic acid in the presence of a base catalyst to form acetylacetone.

2) Butyl Acetate: Butyl acetate may be used as an inert solvent in the synthesis process to dissolve the reactants and facilitate the reaction.

3) Sodium Butoxide (NaOBu): Sodium butoxide acts as a base catalyst in the Claisen condensation reaction between acetone and acetic acid.

4) Inert Solvent (e.g., n-Heptane): An inert solvent such as n-heptane may be used to dilute the reaction mixture and control the reaction conditions.

S.No	Raw Material	Cost (Rs.)	Molecular Mass(g/mol)
1.	Butyl acetate	100/kg	116.16
2.	Sodium Butoxide	350/kg	86.09
3.	N-heptane	70/kg	100.21
4.	Acetone	90/kg	58.08

b. Provide preliminary economic feasibility based on cost of raw materials, solvents and product selling price.

Selling price of Acetyl Acetone is : 2900 Rs/kg (purity 99%)

Molecular mass: 100.16 g/mol

Considering the batch size of 1000 kg and preparing the economic feasibility report

Quantities of Raw Materials Required:

1. NaOBu : 1000kg
2. Buty Acetate: 1000kg
3. Acetone :4000kg (based on stoichiometric ratio provided)

Cost Of Raw Material:

1. NaOBu: 1000 kg * Rs. 350/kg = Rs. 350,000
 2. Butyl acetate: 1000 kg * Rs. 100/kg = Rs. 100,000
 3. Acetone: 4000 kg * Rs. 90/kg = Rs. 360,000
- Total Cost of Raw Materials = Rs. 350,000 + Rs. 100,000 + Rs. 360,000 + Rs. 3590 = Rs. 813,590

Cost Of Solvents:

Inert Solvent (n-heptane):

Quantity used: 50-100 mL

Midpoint of the range: (50 mL + 100 mL) / 2 = 75 mL

Cost of n-heptane: Rs. 70/kg

Density of n-heptane: Approximately 0.684 g/mL (at 20°C)

Mass of n-heptane needed: 75 mL * 0.684 g/mL = 51.3 kg

Cost of n-heptane for 75 mL: (51.3) * Rs. 70/kg = Rs. 3590

Other cost are too associated with it like other Consumables cost, Waste Disposal cost, Labor cost and operating cost.

The process of producing Acetyl Acetone is Profitable.

Profitability:

Final Purity:78%

Overall Yield Of Reaction:83.6%

Selling price of 1000 kg Acetyl Acetone (78% purity):

Revenue = Selling price per 1000 kg (Rs. 2,900,000) * Final Purity (0.78) * Yield (0.836) = Rs. 1,842,240

Profit = Revenue - Total Costs = Rs. 1,842,240 - Rs. 813,590 = Rs. 1,028,650

Observations:

Based on the preliminary analysis, producing 1000 kg of acetylacetone appears profitable with a potential profit of Rs. 1,028,650

References: <https://www.zauba.com/importanalysis-/hs-code-29141990/fp-india/unit-KGS-report.html>

<https://www.sahibindiacorporation.com/acetone-chemical-7556821.html>

<https://dir.indiamart.com/impcat/n-butyl-acetate.html>

<https://dir.indiamart.com/impcat/heptane.html>

<https://www.indiamart.com/proddetail/acetyl-acetone-chemical-24619496212.html>

List the contributions of each author:

- Khushi and Anushri carried out the market research for chemical trade data.
- Khushi and Anushri prepared the use case.
- Harsh looked at economic feasibility.

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Company: National Chemical Limited

CEO: Sidhant Thalor

Report Authors: 1. Anushri Bhargava
2. Komal Kumari

Chemical Formula: $\text{C}_2\text{H}_3\text{ClO}_2$

Chemical Name: MonoChloro Acetic Acid

Use case:

a. What is the use of this compound?

Monochloroacetic acid (MCA) is employed as an intermediate in chemical synthesis, notably in herbicides and surfactants for detergents. Its applications extend to the textile industry for dye fixation, personal care products. MCA's versatility as a reagent in various chemical reactions and its role in water treatment processes highlight its importance across multiple industries.

b. Are there any alternatives to this compound? Name a few.

1. Acetic Acid
2. TCA(Tri Chloro Acetic Acid)
3. Chloroacetyl Chloride

c. Why is this compound superior to its alternatives?

Acetic Acid: Vinegar possesses mild antibacterial properties due to its acidic nature, but it may not be as effective as MCA-based disinfectants in killing certain types of bacteria, viruses, and fungi commonly encountered in household cleaning tasks. MCA-based stain removers for tougher stains than acetic acid.

TCA: TCA is classified as a stronger acid and may pose greater safety hazards compared to MCA. TCA can cause severe skin and eye irritation and is considered more hazardous to handle and store. Production of MCA is also more cost effective than TCA.

Chloroacetyl Chloride : MCA is typically safer and easier to handle compared to chloroacetyl chloride. Chloroacetyl chloride is a highly reactive and corrosive compound that requires careful handling due to its tendency to hydrolyze in the

presence of moisture, releasing hydrogen chloride gas. MCA may have regulatory advantages over chloroacetyl chloride in certain applications due to its lower toxicity and environmental impact.

d. Is this compound imported in India? What is the magnitude of imports?

Monochloroacetic Acid worth \$3,437,959 have been imported. Japan was the largest exporter of monochloroacetic acid accounting for 48.88% of the total imports. Netherlands was the second largest exporter accounting for 30.46% of the total imports of monochloroacetic acid. The month of Mar 2013 accounted for highest number of import shipments. Factors like growing cosmetic and beverage industries in India are expected to positively propel the MCA market in India.

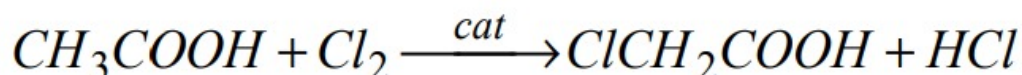
Economic feasibility:

a. What input raw materials are needed for its synthesis (same as reported in the Patent application)?

S No.	Raw material	Cost(in Rs/Kg)	Molecular mass(Kg/kmol)
1.	Acetic Acid	15	60
2.	Chlorine gas	90	70.91
3.	Acetic Anhydride(catalyst)	76.6	102.03
4.	FeCl ₃ (Promoter)	128.8	162.20
5.	Sulphuric Acid	3.3	98

b. Provide preliminary economic feasibility based on cost of raw materials, solvents and product selling price.

Product	Cost(in Rs/Kg)	Molecular mass(Kg/kmol)
MonoChloroAcetic Acid	150	94.5



Economic Feasibility Calculation:

For the production of 1 kmol of MonoChloroAcetic Acid.

Profit = Product Price - All Raw Material Consumption Price

The reaction yield is 89.5%.

$$\text{Profit} = (150 \times 94.5 \times 0.9) - \{(15 \times 60) + (0.5 \times 41 \times 70.9)\} = 12364.3 \text{ Rs/Kmol}$$

So, The profit we get out of selling MCAA is:

$$(12364.3 \text{ Rs/kmol}) / (94.5 \text{ kg/kmol}) = 131.8 \text{ Rs/Kg}$$

References:

Importdata:

<https://www.zauba.com/importanalysis-monochloroacetic+acid/hs-code-29154010-report.htm>

<https://www.chemanalyst.com/industry-report/india-monochloroacetic-acid-43>

List the contributions of each author:

- Anushri has prepared the use case and carried out the market research for chemical trade data.
- Komal looked at economic feasibility based on cost of reactant and selling price of product.

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