Nature of Invention: Chemical molecule and synthesis route

Applicant: CHEMINOVA

Inventors: SHORYA TAMRAKAR (210993), AVNI GOUR (210240)

Chemical Formula: C5H8O2

Chemical Name: METHYL METHACRYLATE

Chemical synthesis routes:

Reaction 1:

Source(patent):

Raw Materials:

- Acetone
- Hydrogen cyanide (HCN)
- Methanol
- Sulfuric acid (H2SO4)
- Ammonium sulphate ((NH4)2SO4)

Reactants:

- Acetone
- Hydrogen cyanide (HCN)
- Water (H2O)
- Sulfuric acid (H2SO4)
- Ammonium sulfate ((NH4)2SO4)
- Methanol

Catalysts:

- Sulfuric acid (H2SO4)

Formation of acetone cyanohydrin (ACH):

Step 1: Acetone + HCN → ACH

- Yield: 70-90%
- Purity: 90-95%
- Time duration: 4-5 hours
- Temperature: 25-35°C
- Pressure: Atmospheric

Hydrolysis of ACH:

Step 2: ACH + H2O + H2SO4 → MAA + (NH4)2SO4

- Yield: 80-90%
- Purity: 98%
- Time duration: 3-4 hours
- Temperature: 35-45°C
- Pressure: Atmospheric
- Endothermic reaction

Esterification of MAA:

Step 3: MAA + MeOH → MMA + H2O

- Yield: 95%
- Purity: 99%
- Time duration: 3-4 hours
- Temperature: 45-55°C
- Pressure: Atmospheric
- Exothermic reaction

Purification of MMA:

Step 4: The MMA formed after the hydrolysis step can be further purified by crystallisation. This can be done by dissolving the MMA in a suitable solvent, such as hot water or ethanol, and then allowing the solution to cool slowly. As the solution cools, the MMA will gradually crystallise out of the solution. The resulting crystals can be filtered, washed, and dried to obtain highly pure MMA.

- Yield: 90-95%
- Purity: 99.5%
- Time duration: 8-12 hours
- Temperature: Room temperature
- Pressure: Atmospheric

Reaction 2:

RAW MATERIAL :

- Isobutylene(C4H8)

CATALYSTS:

- Zeolites

- SAPO molecular sieve

REACTANTS:

- Isobutylene
- Methacrolein
- Methacrylic acid

Step1 - Dehydrogenation of isobutylene

Isobutylene (C4H8) is dehydrogenated to methacrolein (C4H6O) and hydrogen gas (H2).

$C_4H_8 \rightarrow C_4H_6O + H_2$

Conditions:

- Temperature - 250-350°C
- Pressure - 0.1-5 MPa
- Catalyst - solid catalyst such as a zeolite or SAPO molecular sieve.
- Exothermic process

STEP 2
Oxidation of methacrolein:

Methacrolein is then oxidized with an oxygen-containing gas, such as air, to produce methacrylic acid (C4H6O2).

$C_4H_6O + 1/2\ O_2 \rightarrow C_4H_6O_2$

- Temprature - 200-250°C
- Pressure - 0.1-2 MPa
- Catalyst - copper or cobalt compound

STEP 3
Esterification of methacrylic acid:

Methacrylic acid is esterified with isobutylene to produce methyl methacrylate (C5H8O2) and water (H2O).

$C_4H_6O_2 + C_4H_8 \rightarrow C_5H_8O_2 + H_2O$

Conditions:

- Temperature - 150-250°C
- Pressure - 0.1-10 MPa
- Catalyst - zeolite or SAPO molecular sieve.

STEP 4:Purification of the product

The product stream is then further purified through various techniques, such as distillation, crystallization, or adsorption, to obtain the desired purity level of the product.

Generally, the temperature is kept below the boiling point of MMA (around 101°C at atmospheric pressure) to prevent decomposition and side reactions.

Overall:

- Temperature - 240°C
- Pressure - 1 MPa
- Reaction time - 4 hours
- Yield - 90%

References: https://patents.google.com/patent/US20020188151A1/en

https://patents.google.com/patent/EP0941984A2/en EP0941984A2

List the contributions of each author:

SHORYA TAMRAKAR (210993) carried out the literature search and find the reaction steps, and product yield as well as found necessary separation steps to achieve desired product purity for preparation of MMA from method one.

AVNI GOUR (210240) carried out the literature search and found the reaction steps, and product yield as well as found necessary separation steps to manufacture MMA from method two.

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Name	Roll No	Signature
CEO Name: Zainab Fatima	211211	Zainab
First author Name: Shorya Tamrakar	210993	Shorya
Second author Name: Avni Gour	210240	Avni