



Mannar Thirumalai Naicker College (Autonomous)

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ORGANIC CHEMISTRY – II

Mechanism of Benzoin condensation reaction & Claisen condensation reaction

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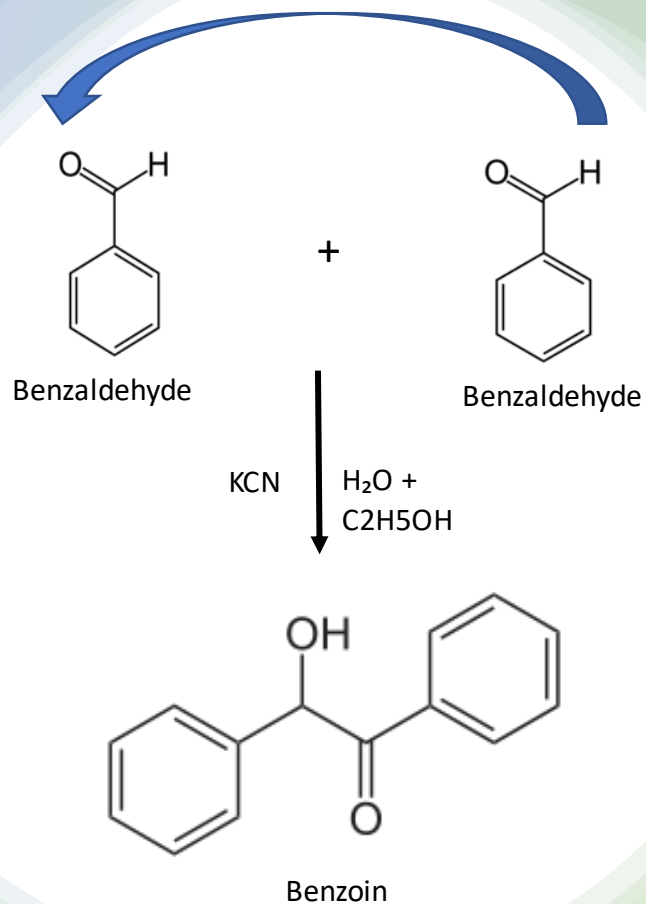
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Mechanism of Benzoin Condensation

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- **General Principle**
- **Requirements of the Reaction**
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- **Applications**

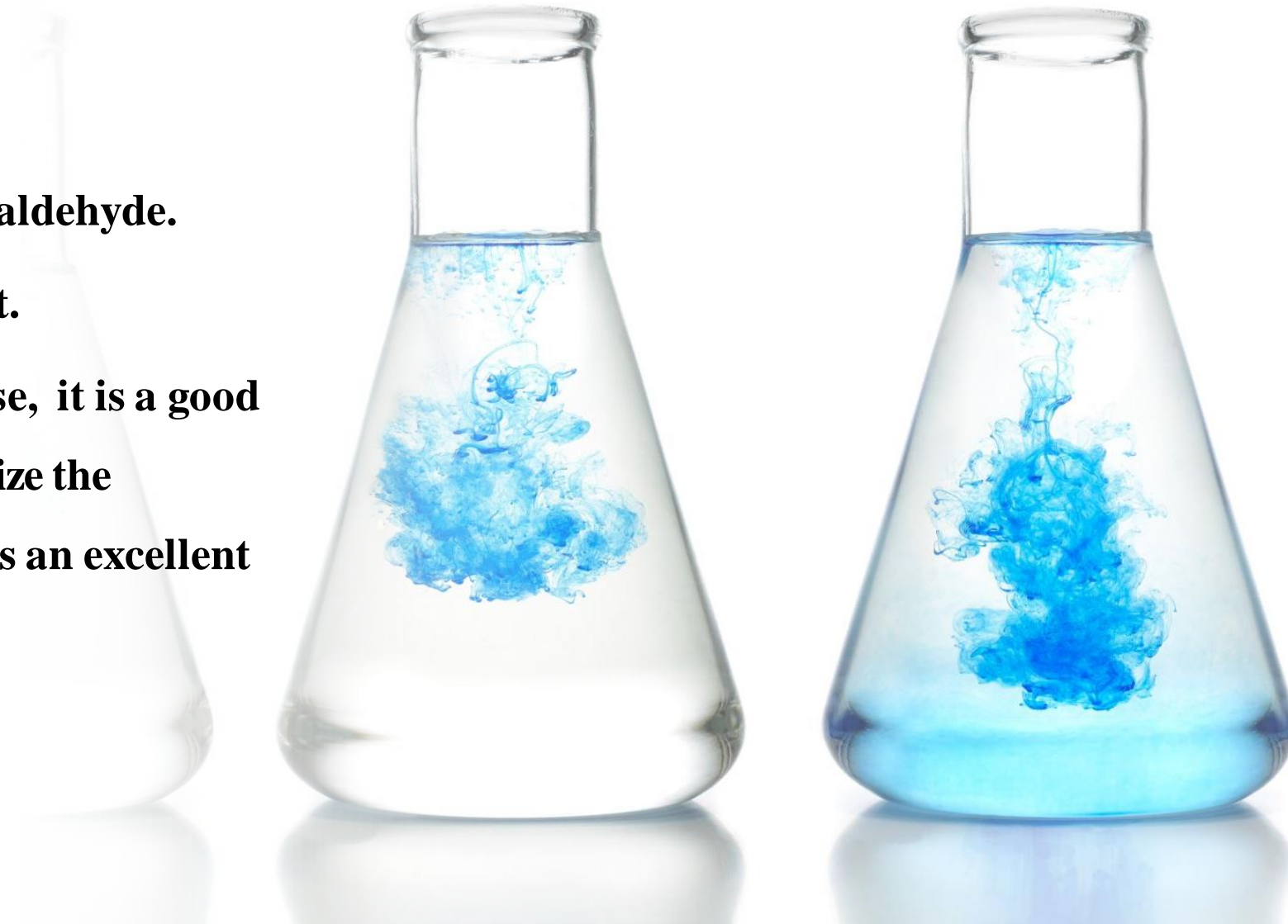
General principle



- ❑ The benzoin condensation is condensation between two molecules of benzaldehyde to form benzoin in the presence of cyanide catalyst (e. g ; NaCN and KCN) or thiamine (vitamin B).
- ❑ The structure of benzoin is that of ketone.
- ❑ It consists of acetophenone bearing hydroxy and phenyl substituents at the alpha position (α - hydroxyl ketone).
- ❑ Its IUPAC name is 2-hydroxy-1,2-diphenylethanone with a molecular mass of 212.24 g/mol.
- ❑ A cyanide ion usually catalyses benzoin condensation.

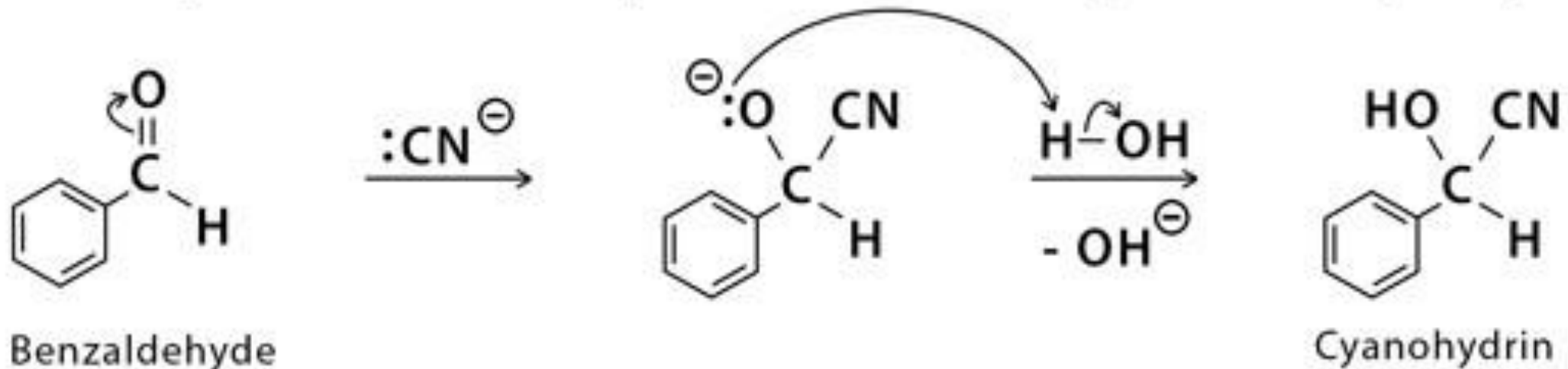
Requirements of the reaction

- ❑ Two molecules of benzaldehyde.
- ❑ Cyanide ion as catalyst.
- ❑ Cyanide is used because, it is a good nucleophile, can stabilize the intermediate ion, and is an excellent leaving group.



Reaction mechanism

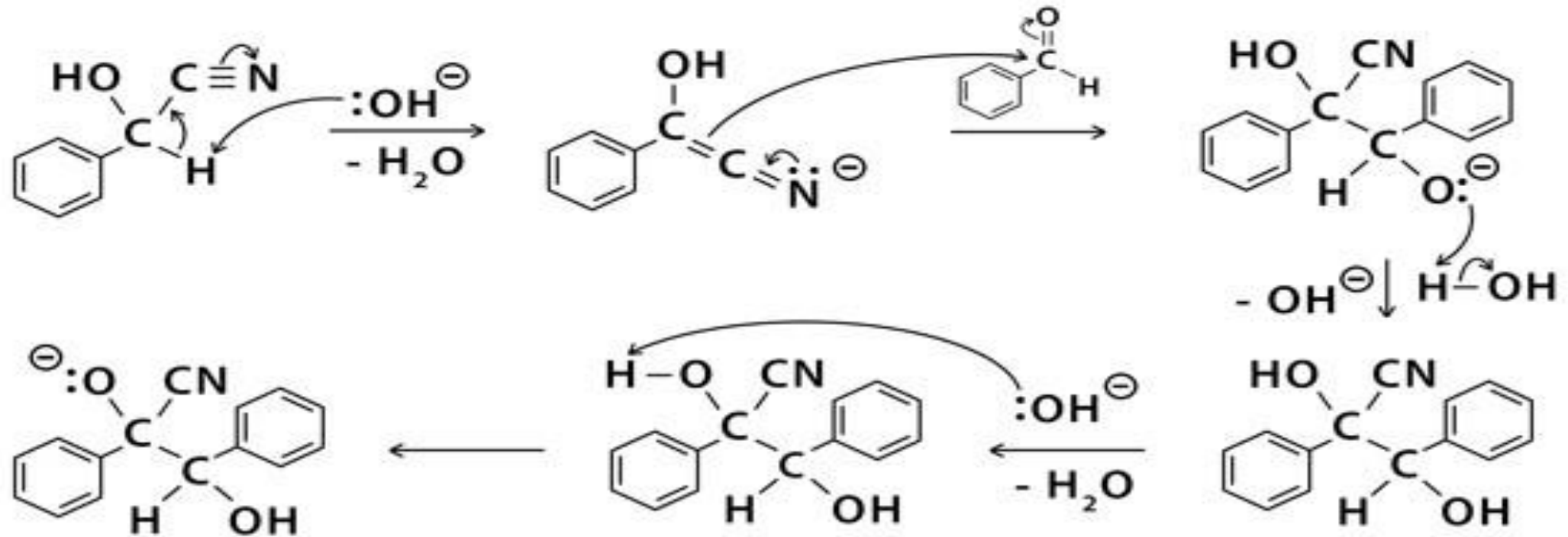
Step 1: Nucleophilic addition of a cyanide with benzaldehyde to form cyanohydrin



- The first phase of the process includes the reaction of cyanide ions with the benzaldehyde to form the product called cyanohydrin. In this step, the cyanide ion or sodium cyanide takes part in the nucleophilic addition reaction, and it is a reversible reaction. The cyanide ion helps the reaction to occur by acting as a nucleophile and facilitating the abstraction of protons, thus forming cyanohydrin. The cyanide ions serve as a catalyst in the reaction.

Reaction mechanism

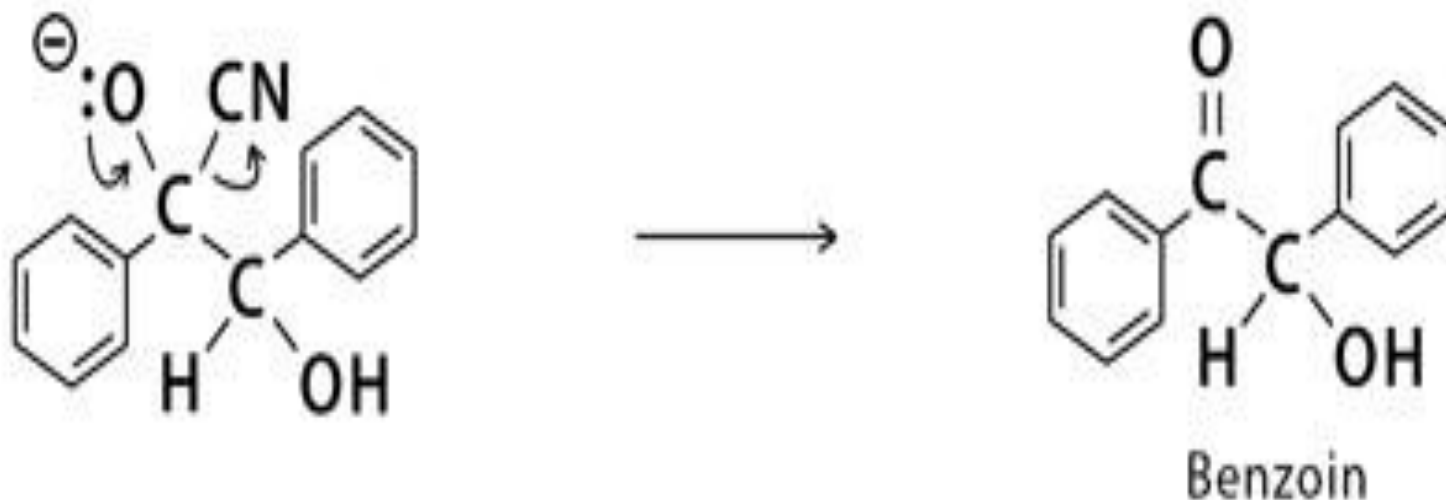
Step 2: Condensation reaction between the cyanohydrin and a second benzaldehyde



- The second step is the condensation reaction that occurs between the cyanohydrin and the benzaldehyde.

Reaction mechanism

Step 3: Rearrangement reaction removing the cyanide group resulting in a benzoin



- In the third step, rearrangement occurs and also the removal of the cyanide ions occurs resulting in the formation of benzoin. The Rearrangement process results in the reversal of polarity of the carbonyl group, later adding to the second group of carbonyl atom in the second nucleophilic addition.

Applications

- ✓ Benzoin is applied on skin to protect it from allergy.
- ✓ Benzoin can be applied skin fissures, fever blisters as an antiseptic.
- ✓ Benzoin is used for treatment of asthma and common colds.
- ✓ Benzoin is used in military also to prevent loss of skin.
- ✓ Benzoin condensation reaction is used for the synthesis of various organic compounds and in reactions.
- ✓ This reaction is used in synthesis of heterocyclic compounds. It is also used to extend aliphatic form of aldehydes.
- ✓ This reaction is used in polymer chemistry.



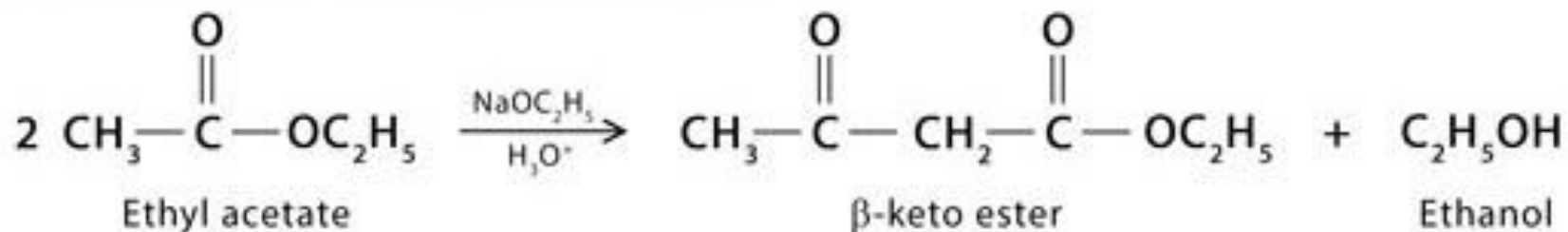
Mechanism of Claisen Condensation

CONTENTS

- **General principle**
- **Reaction Mechanism**
- **Applications**

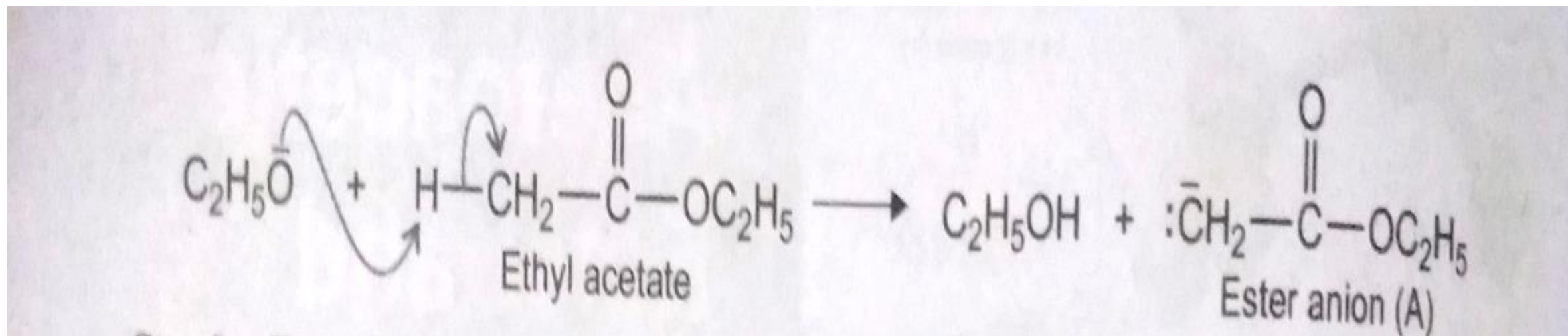
General principle

- ❑ The Claisen condensation reaction is an organic coupling reaction that results in the formation of a C-C bond between either a single ester and one carbonyl compound or between two esters.
- ❑ The reaction proceeds when a strong base is present and the product of the reaction is a beta-keto ester or a beta-diketone.



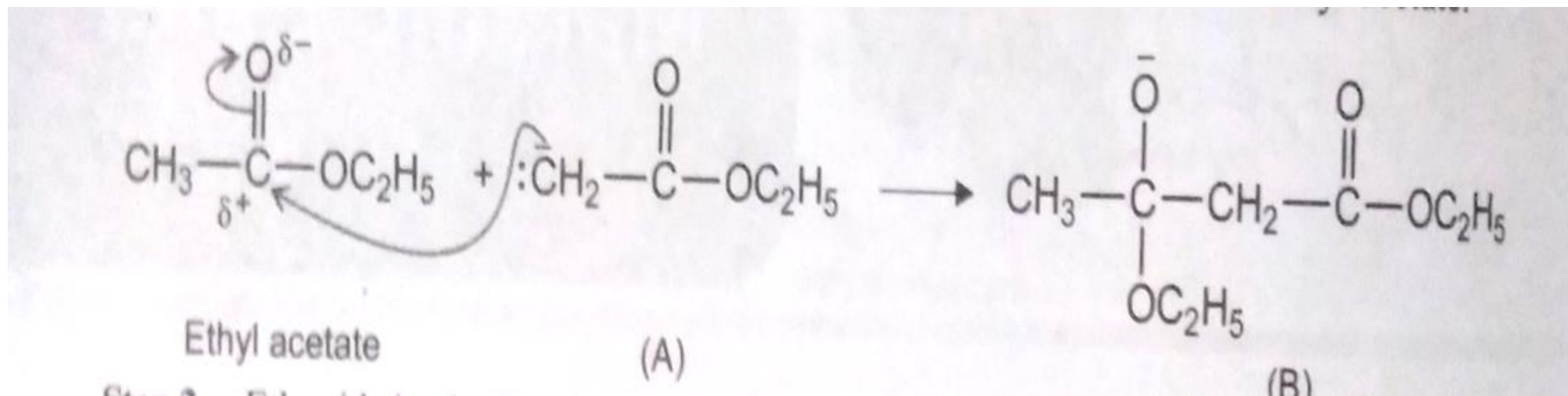
Reaction mechanism

Step – 1 Ethoxide ion (from C₂H₅ONa) attacks ethyl acetate to give ethyl alcohol and the ester anion.



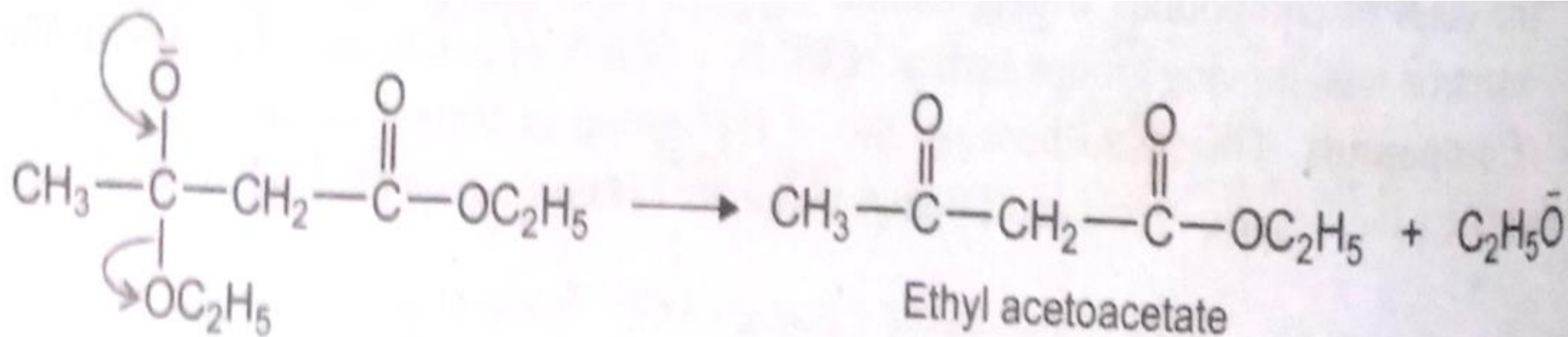
Reaction mechanism

Step – 2 Ester anion attacks the carbonyl group of a second molecule of ethyl acetate.



Reaction mechanism

Step-3 Ethoxide ion is eliminated



(B)

Applications

- It is a critical method for the synthesis of β -ketoesters or β -diketones in organic chemistry and is frequently used for the synthesis of several compounds, such as medicines, flavorings, and fragrances.
- The Claisen Ester Condensation offers several benefits. Carbon-Carbon Bond Formation: The Claisen Ester Condensation allows for the efficient construction of new carbon-carbon bonds, an indispensable reaction in organic synthesis.

References:

- March, J., *Advanced Organic Chemistry*, Wiley Eastern Limited, 1994.
- R.K. Bansal, *Organic Reaction Mechanism*, Wiley Eastern Limited, New Delhi, 1993.
- I.L. Finar, *Organic Chemistry*, ELBS Longmann, Vol. I & II, 1984.



THANK YOU

