

Study Notes On Claisen Condensation Reaction



CLAISEN CONDENSATION

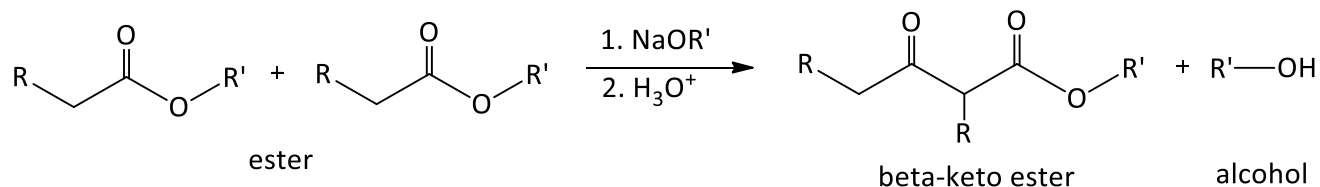
In the Claisen Condensation reaction, self-condensation occurs between two molecules of an ester containing α -hydrogen or between one ester and another carbonyl compound in presence of a strong base to form β -keto ester or β -diketone.

Note:

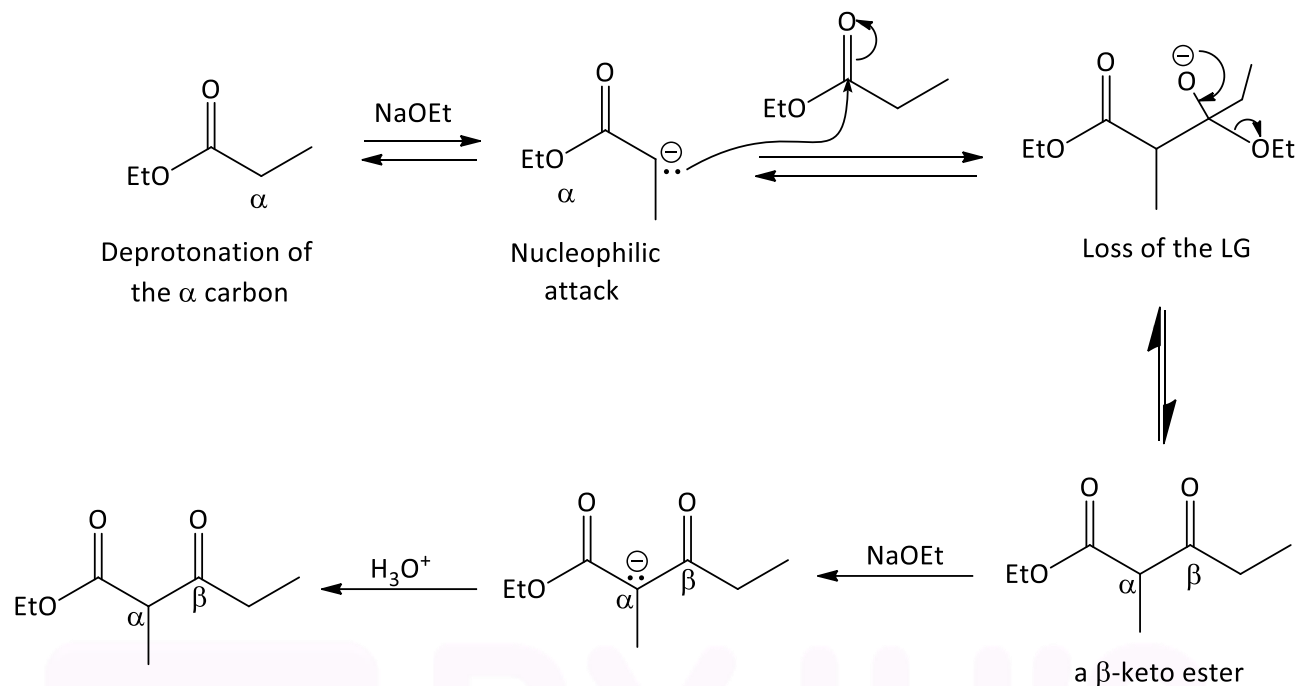
1. Strong base such as – sodium ethoxide is used.
2. The driving force in this reaction is the formation of stabilized anions of β -keto ester.
3. To increase the yield, strong bases are used instead of sodium ethoxide, such as – sodium amide, sodium hydride, etc.
4. The intramolecular Claisen condensation is known as Dieckmann condensation.
5. This reaction is termed as condensation reaction because it eliminates a small amount of alcohol as a side product.
6. During this reaction, a new Carbon-Carbon double bond is formed to produce a β -keto ester.
7. To avoid transesterification side products, the alkoxide base possesses the same alkyl group as in the alkoxy group present in ester starting material.
8. This reaction is driven by Le-Chatelier's principle. Thus, a product will not form if it does not contain an α -hydrogen acidic enough to react completely with the reaction base.

Hence, the ester starting compounds must have at least two α -hydrogen for this reaction to occur; out of which one is removed to form ester enolate and the other gets removed and drives the reaction forward.

General Reaction-



Reaction Mechanism-

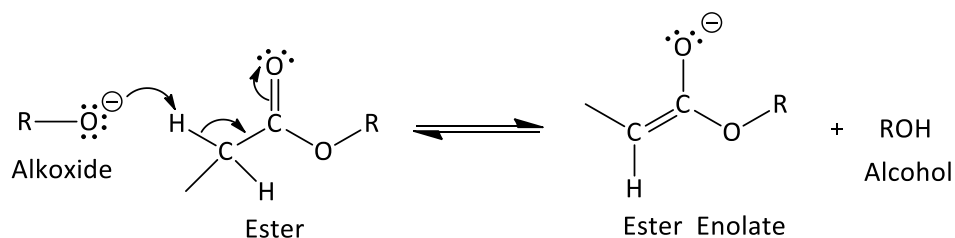


The β -keto ester has a very acidic proton which is removed by the base. Therefore, an acidic workup is needed

This mechanism is similar to saponification reaction, and it could be understood step-by-step as follows-

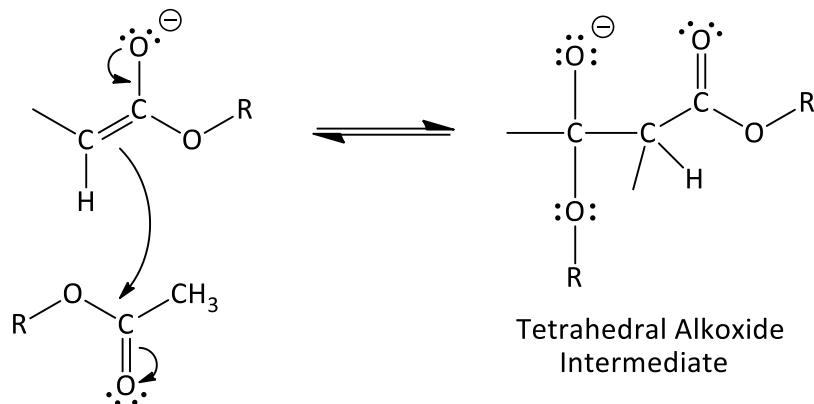
1. Enolate formation

The alkoxide base removes an alpha-hydrogen from the ester to form a nucleophilic ester enolate ion.



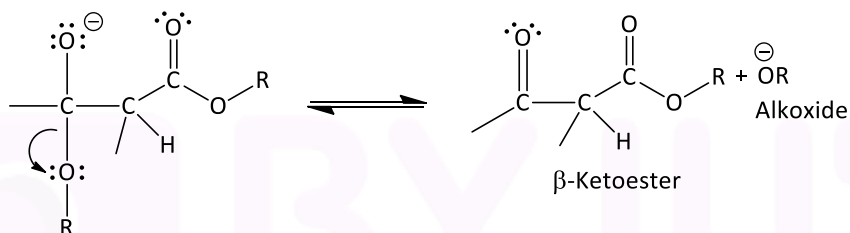
2. Nucleophilic attack

The enolate nucleophile so formed adds to the carbonyl carbon of a different ester, forming a tetrahedral alkoxide intermediate.

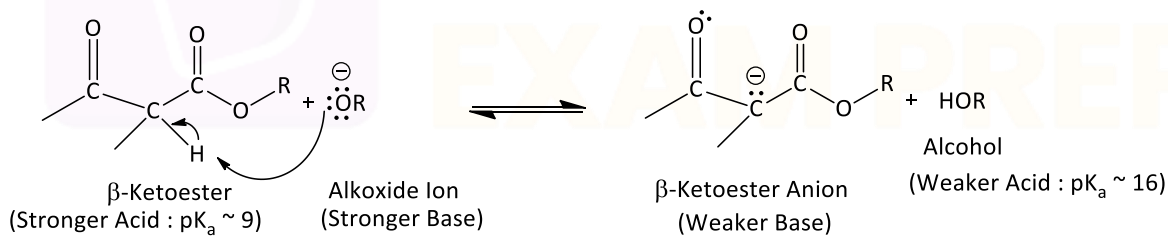


3. Removal of leaving group

The alkoxide then reforms the carbonyl to form a beta-ketoester by eliminating the $-OR$ as leaving group.

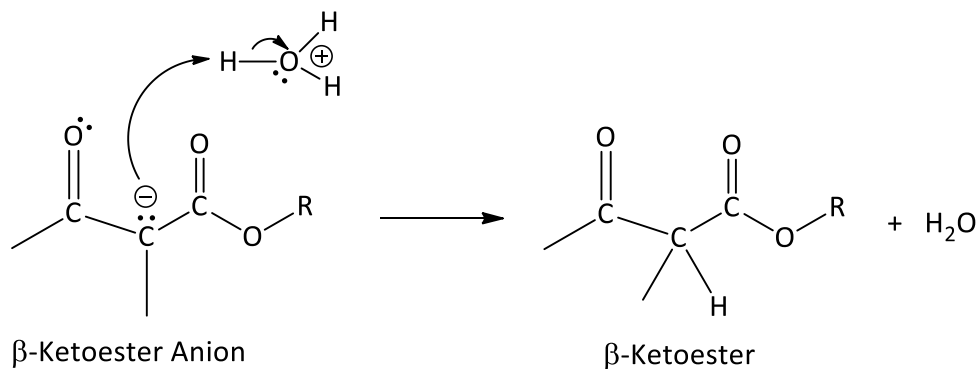


4. Deprotonation



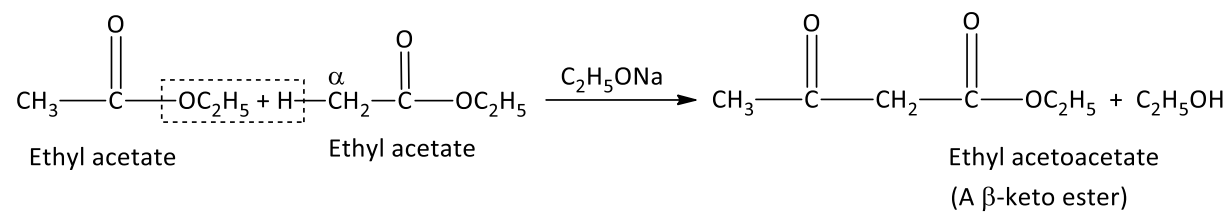
5. Protonation

The enolate is protonated in an acid work-up to form the neutral beta-ketoester product.



Note: Stereochemistry = a racemic mixture of enantiomers will form.

Example-



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