

Introduction:

The crossed aldol condensation is an important class of organic reaction for the generation of new carbon-carbon bonds (Pitre, Stokes & Misna, 2021). During this reaction, in the presence of a base, two different compounds containing carbonyl groups react to form the target molecule. This experiment described how two different carbonyl functional group-containing compounds, including Cinnamaldehyde and Acetone, react to form a ketone that shows high conjugation.

Theoretical Background:

Carbons adjacent to carbonyl groups (α carbons) possess slightly acidic hydrogens. When these types of compounds are treated with a strong base, alpha-hydrogens are removed easily, and an enolate is formed. This enolate compound is resonance-stabilized and acts as a nucleophile. This nucleophile attacks the carbonyl group of other compounds, and a new carbon-carbon bond is formed. The newly formed compound is known as an aldol compound, as it contains both an alcohol and an aldehyde functional group. After elimination of water, a conjugated α,β -unsaturated carbonyl compound is formed, which is thermodynamically favored due to the extended conjugation.

Reaction:

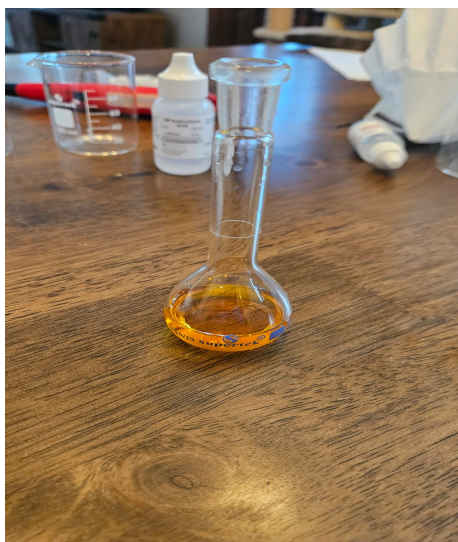
In this experiment, one equivalent of acetone reacts with 2 equivalents of cinnamaldehyde in the presence of strong base NaOH and ethanol. As a result, a highly conjugated ketone product is formed with extended aromatic conjugation.

Safety Considerations:

- (I) Must wearing safety goggles during the experiment.
- (ii) Wear protective gloves which is made of latex, nitrile or rubber during perform the experiment.
- (iii) Carefully handle 1M NaOH because it cause burn when contact with skin.
- (iv) If NaOH comes touch with skin then immediately wash the affected area with cold water.
- (v) Handle Cinnamaldehyde and Acetone in a well ventilated area.

Result:

(a)



(b)



Image 1: Few pictures of the flask over the 10 minutes

3.5 mL of cinnamaldehyde and 1.0 mL of acetone were reacted in the presence of 91% isopropanol (5 mL) and 1 M NaOH (20 drops) as a base catalyst, undergoing the crossed aldol condensation (Image 1). A pale yellow precipitate was formed after vigorous swirling for 10

minutes at room temperature. After cooling the mixture by using an ice bath, a larger amount of solid was crystallized. Then vacuum filtration was performed, and the product was washed with ice-cold water. The resulting crude product was air-dried for several hours and obtained a pale yellow crystalline solid(Image 2). The mass of product was 0.11 oz.

(a)



(b)



Image 2: Pictures of the product

Discussion:

This experiment successfully demonstrated a crossed aldol condensation reaction between two different carbonyl compounds, which formed a conjugated α,β -unsaturated ketone. This condensation reaction was carried out in the presence of base NaOH, which initially deprotonated acetone and formed an enolate, which acted as a nucleophile in this reaction. This nucleophile attacked the more electrophilic carbonyl carbon of Cinnamaldehyde and formed the

desired products. As Cinnamaldehyde, due to the lack of α -hydrogens, it is unable to generate its own enolate. This helped to act as an electrophile and undergo a crossed (mixed) aldol reaction rather than the self-condensation of acetone.

Conclusion

This experiment successfully demonstrated the crossed aldol condensation reaction between two different carbonyl functional group-containing compounds, including Cinnamaldehyde and Acetone, which react and form a ketone that shows high conjugation. The reaction illustrates important concepts in organic chemistry, including enolate formation, nucleophilic addition to carbonyls, and the stability provided by conjugated systems.

References

Pitre, D., Stokes, S., & Misna, D. (2021). Crossed Aldol Condensation. *Journal of Chemical Education*, 98(7), 2403-2410. DOI: 10.1021/acs.jchemed.0c01262