

# Experiment 6 - Aldol Condensation

## OBJECTIVE

To provide experience with Aldol condensation, a useful reaction to prepare conjugated carbonyl systems.

## INTRODUCTION

Hydrogen atoms that are located on a carbon adjacent (alpha) to a carbonyl group are acidic and can be removed by base. The acidity is due to the fact that the carbanion produced is stabilized by resonance with the carbonyl group (1 and 2). The carbanion is a nucleophile and is capable of adding to electrophilic centers such as the carbon of the carbonyl group in aldehydes and ketones. The result of such a reaction is the formation of a beta-hydroxy carbonyl compound (3). In cases where there are aromatic substituents, these initial products undergo dehydration to yield the conjugated system (4).

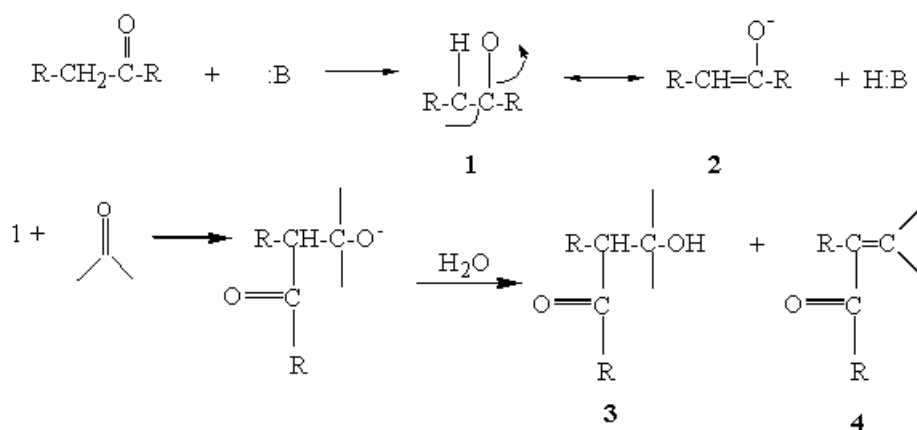


Figure 1

## PRE-LAB

Complete the pre-lab assignment in WebAssign.

## Preparation of Dibenzalacetone

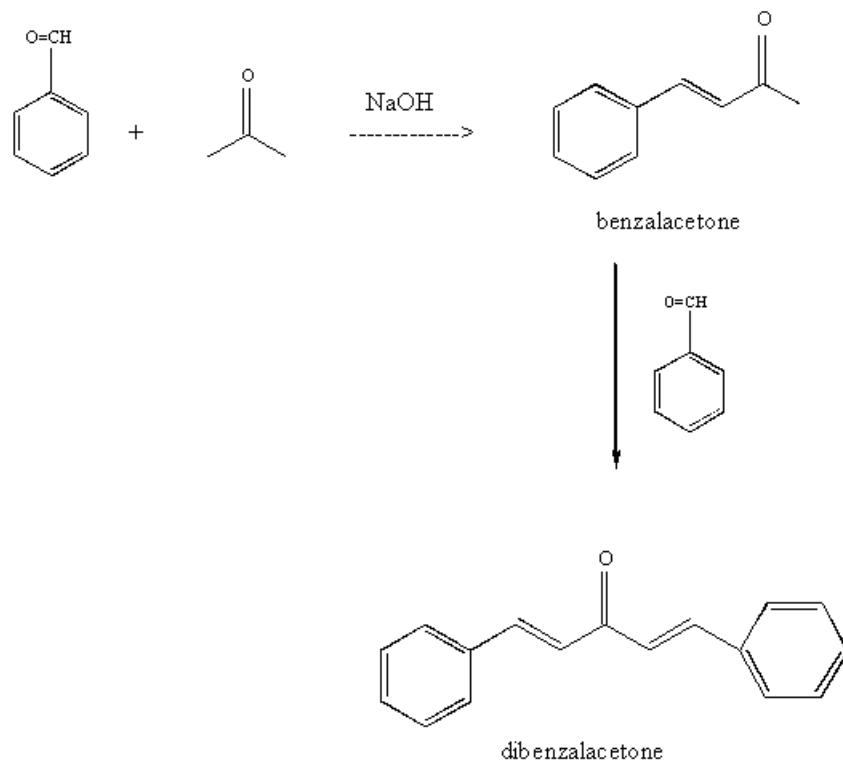


Figure 2

The preparation of dibenzalacetone (1,5-diphenyl-1,4-pentadien-3-one) is an example of an aldol condensation in which the ketone, acetone, possesses two sets, albeit equivalent, of alpha-hydrogens. The original product, benzalacetone, contains a set of alpha-hydrogens which can be used to effect another nucleophilic substitution onto a second benzaldehyde molecule. By using a 2:1 molar ratio of benzaldehyde to acetone, one can obtain disubstitution as the principal product. What is the mechanism of this reaction?

## PROCEDURE

In a small Erlenmeyer flask, mix 2 mL of the sodium hydroxide solution with 2 mL of 95% ethanol.

**CAUTION:** The NaOH solution is about 20%; avoid contact. *Wash hands after use!*

To the resulting solution, add 0.3 mL of acetone followed by 0.8 mL of benzaldehyde (use dispensing pipets). Swirl the flask intermittently for 15 min, then isolate the product using vacuum filtration and washing the precipitate with a small amount of cold water followed by a small amount of chilled 95% ethanol. Allow the sample to dry (since an aqueous solution was used, this may take some time), determine the melting point, crude yield and percentage yield. The product may be recrystallized from 95% ethanol.

## IN-LAB QUESTIONS

Download and print the following worksheet. You will use this worksheet to record your answers to the In-Lab questions.

## Questions

Record the following data.

**Question 1:** Amount of benzaldehyde \_\_\_\_\_ mL, \_\_\_\_\_ g, \_\_\_\_\_ mol

**Question 2:** Amount of acetone \_\_\_\_\_ mL, \_\_\_\_\_ g, \_\_\_\_\_ mol

**Question 3:** Theoretical Yield of Product \_\_\_\_\_ mol, \_\_\_\_\_ g

**Question 4:** Actual Yield of Product \_\_\_\_\_

**Question 5:** Percentage Yield \_\_\_\_\_

**Question 6:** Melting Point of Product \_\_\_\_\_ (observed), \_\_\_\_\_ (reported)

**Question 7:** Record your calculations.

**Question 8:** Record the mechanism of reaction.