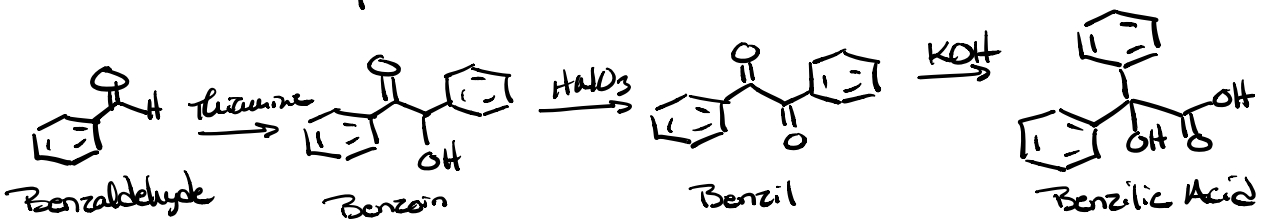
Multistep Formal Report



Abstract

what was done & what was found.

Benzilic acid was synthesized in three steps from benzaldehyde in a multistep reaction. Benzaldehyde was reacted with thiamine hydrochloride to produce benzoin. ....

Introduction

Stimulates interest. Sets stage by looking at prior work. What is important, what is the focus of the work?

⇒ need for multistep synthesis to make complicated molecules.

⇒ Taxol, one of first cancer drugs

multistep = "Total Synthesis"

last ¶ non-technical overview.

⇒ Restates what this work is going to present.

Methods & Materials

⇒ materials & Equipment list

⇒ all chemicals used

⇒ Instrumentation

Meltemp

digital thermometer

FTIR

IR Software

⇒ method

⇒ Benzoin

Thiamine hydrochloride (0.30 g, x mmol) was added to a 25-mL erlenmeyer flask, and dissolved in 0.45 mL DI water. Ethanol (95%, 3 mL) was added and then 0.9 mL of 2M aqueous sodium hydroxide was added . . .

Benzoin (x g, y mmols, z %, MP, FTIR)

⇒ Benzil

⇒ Benzilic Acid

Results Section

one idea

	MP	% Yield	FTIR (cm^{-1})	Characterization
Benzoin	x-x °C	y %	3400 cm^{-1} 1680 cm^{-1}	hydroxyl Ketone
Benzil	x-x °C	y %	1690 cm^{-1} 1660 cm^{-1}	Ketone C=C
Benzilic Acid	x-x °C	y %	3500 cm^{-1} 3400 cm^{-1} 1690 cm^{-1}	hydroxyl Carboxylic acid Carbonyl

overall yield ~ 5%

$$\frac{\%y \text{ benzoin}}{100} \times \frac{\%y \text{ benzil}}{100} \times \frac{\%y \text{ benilic acid}}{100} \times 100 = \%\text{ overall}$$

TP for each material that gives results in paragraph form. Here you can also include a physical description of the material

Discussion Section Outline

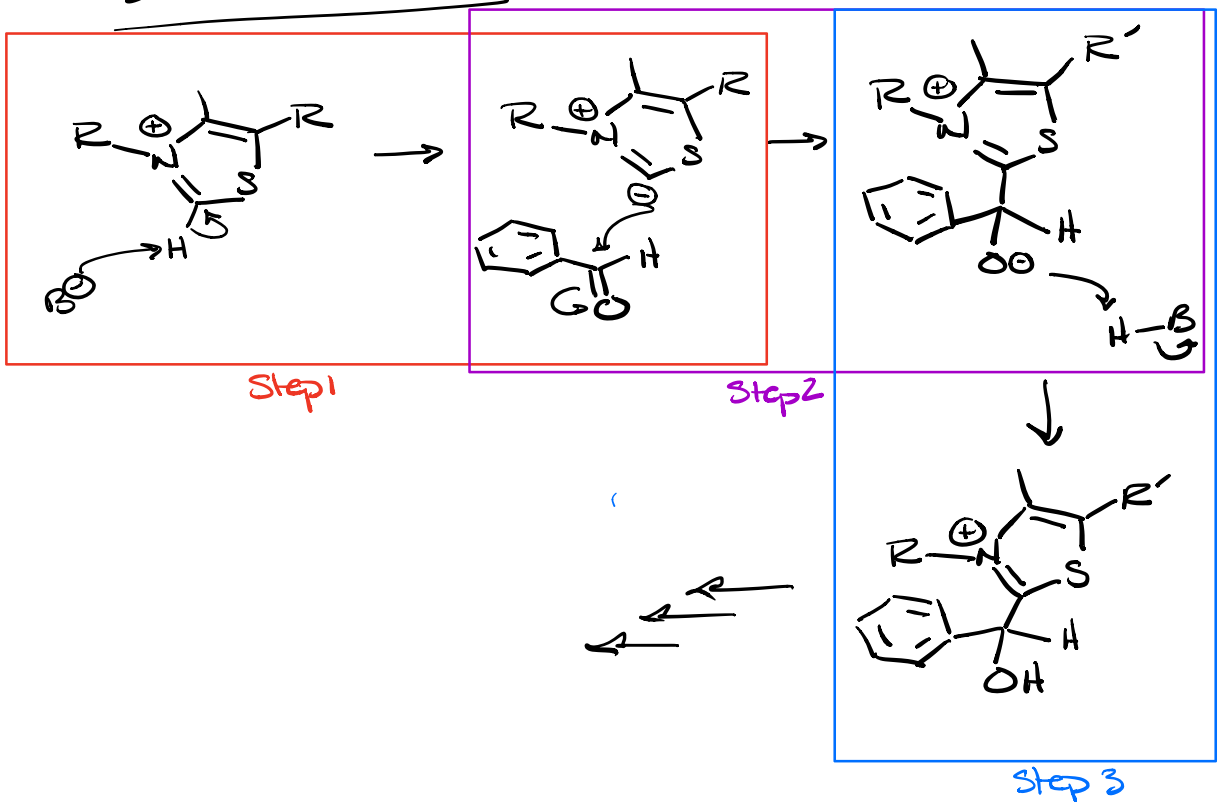
⇒ Break down by reaction

Benzoin { – mechanism
– Characterization

Benzil { – mechanism
– Characterization

⋮

Benzoin mechanism



The formation of benzoin from benzaldehyde is catalysed by thiamine hydrochloride. The first step in this reaction is the deprotonation of thiamine hydrochloride by hydroxide ion.

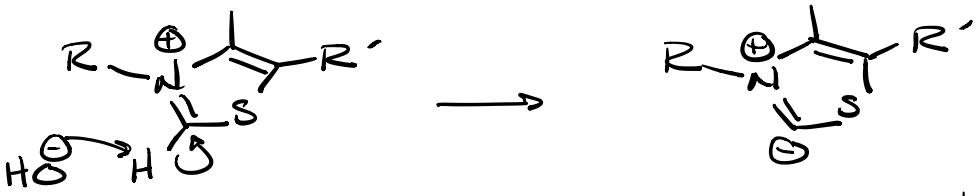


Figure 1. The deprotonation of thiamine · HCl

⇒Next TP address the why

Thiamine hydrochloride is deprotonated at the carbon between the nitrogen and sulfur. The resulting anion is stabilized by the adjacent nitrogen cation forming a stable ylide[1]. The ylide is a carbon nucleophile and proceeds to conduct a nucleophilic attack on benzaldehyde.

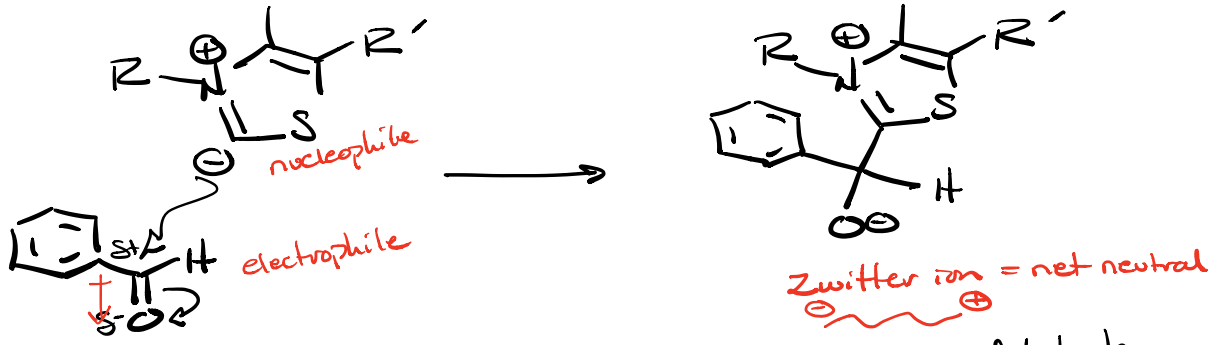


Figure 2. nucleophilic attack on benzaldehyde

[1] Camara et. al. P

TP ⇒ talks about the step mechanics & the why

⋮

⇒ next after mechanism is characterization

- % Yied (High or low, why?)
- agree? { - MP (corresponds to lit, off-from Lit, why?)
  - FTIR (Compare transformation from starting material. Comparison w/ literature)

⇒ move on to benzil & Repeat

- mechanism
- Characterization

⇒ move on to benzilic acid

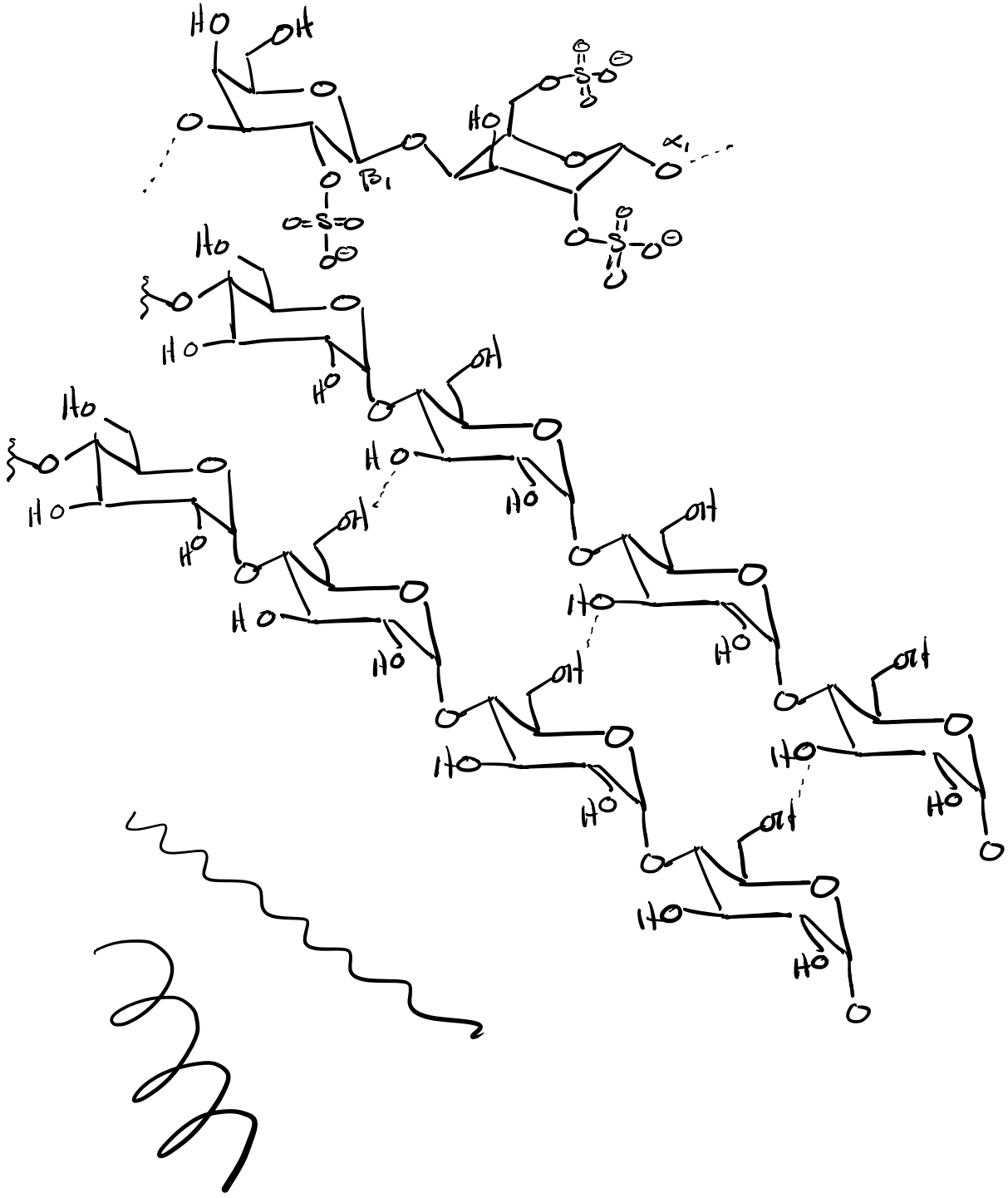
⇒ Conclusion

- Restatement of abstract & the major findings

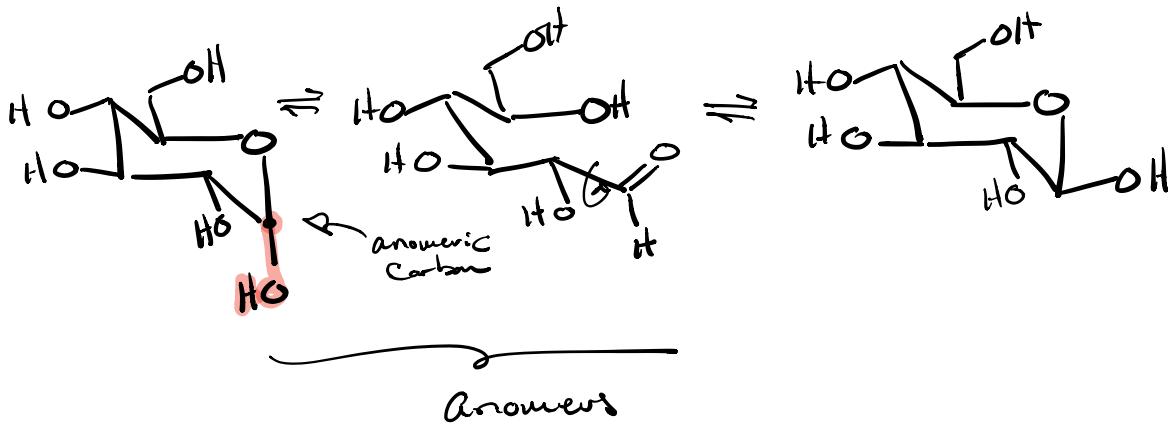
⇒ Separation Schemes (may be in Lab Notes)

⇒ lab notes

⇒ Spectroscopy (may be in the discussion as a figure)



Hemi acetals



Anomers