

Honors Cup Synthetic Proposal

Section: 216H.221, Group C

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Title: Three-step synthesis of *trans*-cinnamaldehyde from cinnamic acid

Introduction

Trans-cinnamaldehyde is the molecule that is responsible for cinnamon's characteristic taste and smell. It is found in the bark of cinnamon trees. Typical cinnamon-scented products contain only a few tenths of a percent of this very strong compound. Cinnamaldehyde is also used as an agricultural fungicide.

Overall Synthetic Reaction Scheme

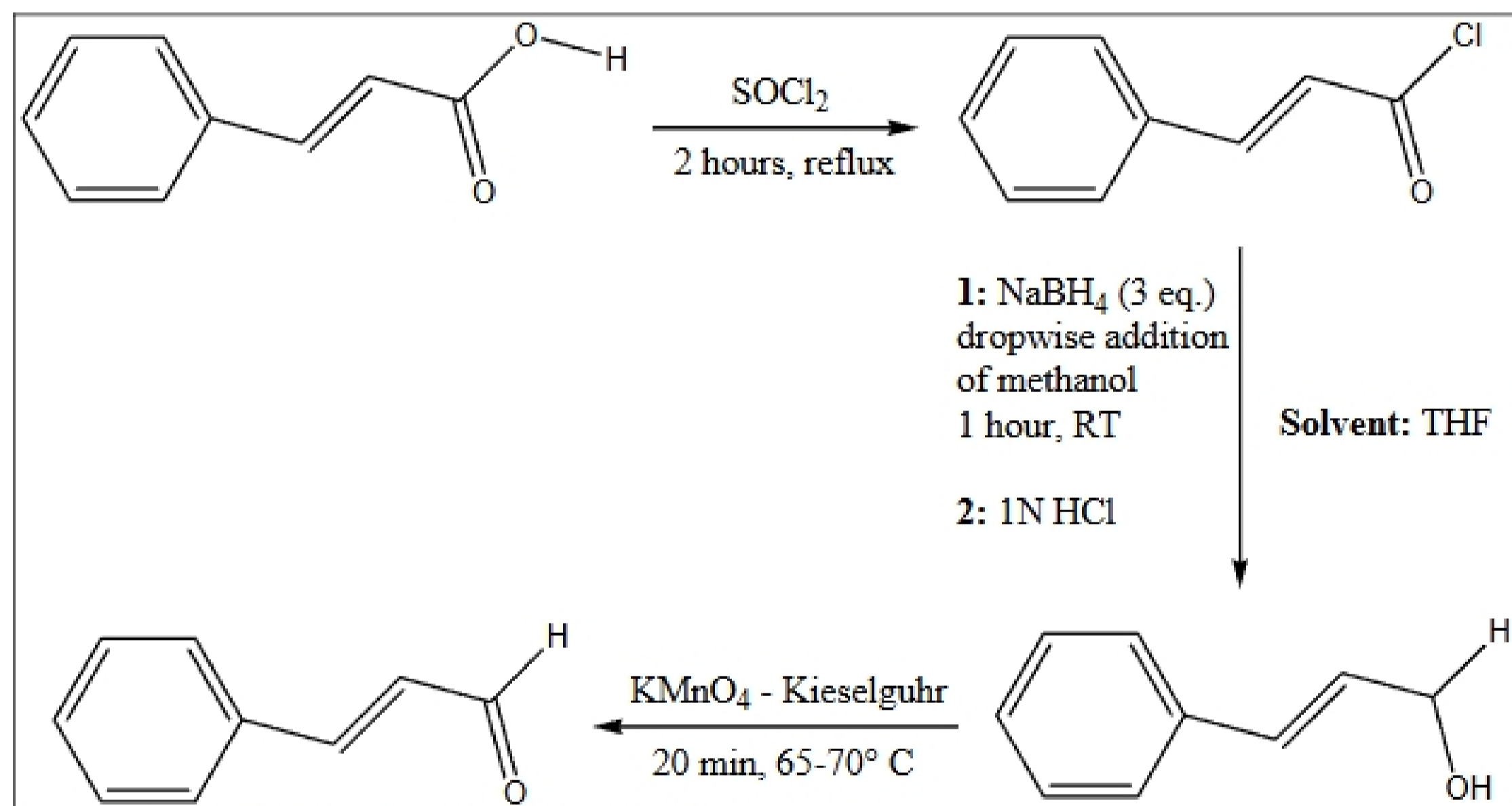


Figure 1: Overview of three-step *trans*-cinnamaldehyde synthesis

Synthetic Transformation I

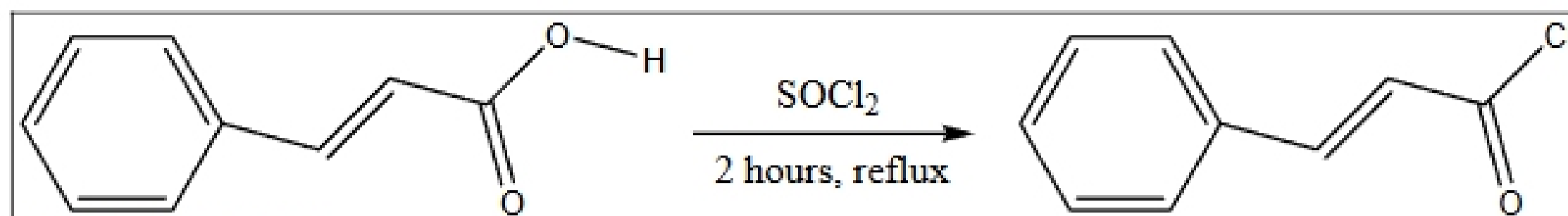


Figure 2: Transformation I

Experimental I

The first step of this synthesis involves the transformation of cinnamic acid to its acyl chloride form, cinnamyl chloride. This well-known reaction^{1,2} is performed by heating cinnamic acid (2 g, 13.50 mmol) and freshly distilled thionyl chloride (2.29 mL, 31.5 mmol) under reflux and stirring for two hours. The excess thionyl chloride is then distilled off. Yields range from 58 to 87%¹. Even in the case of 58% yield, enough product will be formed to reach our target goal of 0.5 g of *trans*-cinnamaldehyde. Yields for the remainder of this proposal will reflect the maximum 87% yield.

Expected yield: 87%, 1.79 g

Safety, Disposal and Green Issues of Transformation I

Cinnamic acid is an eye, respiratory, and skin irritant and should be handled under a fume hood. In case of eye contact, wash with plenty of water for at least 15 minutes and seek medical advice. Be sure to wear suitable clothing when handling cinnamic acid. In case of swallowing, wash mouth out with water *if person is conscious* and call a physician. If cinnamic acid comes in contact with skin, wash with soap for at least 15 minutes. If inhaled, remove person to fresh air and give artificial respiration in case the person stops breathing. In case of ignition, use carbon dioxide, dry chemical powder, or appropriate foam. Cinnamic acid emits toxic fumes under fire conditions and appropriate breathing apparatus and clothing should be worn during fire fighting. Cinnamic acid should be disposed of by mixing with a combustible solvent. Solution should then be burned in a chemical incinerator with afterburner and scrubber.

Thionyl chloride is corrosive and reacts vigorously with water. Contact with water also releases toxic gas. Contact of this gas with metal surfaces can form explosive hydrogen gas. Thionyl chloride is harmful if inhaled and if swallowed. Skin contact can also produce severe burns, and this compound also has an unpleasant odor. In case of skin or eye contact, inhalation, or ignition, follow instructions given for cinnamic acid. The same applies for ingestion, and *by no means* induce vomiting. Thionyl chloride may decompose into harmful carbon dioxide, carbon monoxide, and hydrogen chloride gasses over extended periods of time. Disposal instructions for thionyl chloride are the same as cinnamonic acid disposal (above).

Cinnamyl chloride is highly toxic and may cause sensitization and/or burns on skin contact. In case of ingestion, skin or eye contact, or ignition, follow instructions given for cinnamic acid. Excessive inhalation of cinnamyl chloride causes respiratory depression and can be fatal.

Disposal instructions for cinnamyl chloride are the same as cinnamonic acid and thionyl chloride disposal (above).