Green preparation of benzaldehyde derivatives using an oxoammonium nitrate salt

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INTRODUCTION

- Benzaldehyde derivatives are a class of compounds that contain a six-membered carbon ring and a carbonyl group (C=O) as shown in Figure 1.
- These molecules are essential to pharmaceutical, fragrance, and food industries. For example, benzaldehyde is commonly used for its distinct almond flavor.[1]

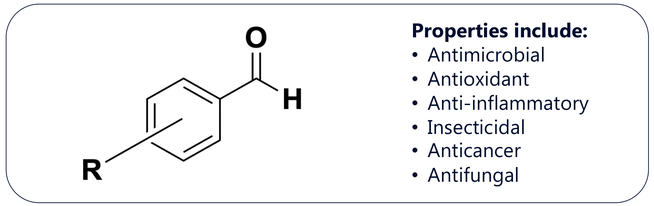

Figure 1. Structure and applications of benzaldehyde derivatives.[2,3,4]

- Benzaldehyde and its derivatives are usually prepared using oxidative reactions.
- Traditional oxidation methods often use highly toxic reagents that cause significant harm to the environment when disposed of.[5]
- We aim to perform this reaction in a cleaner, greener, and safer manner.

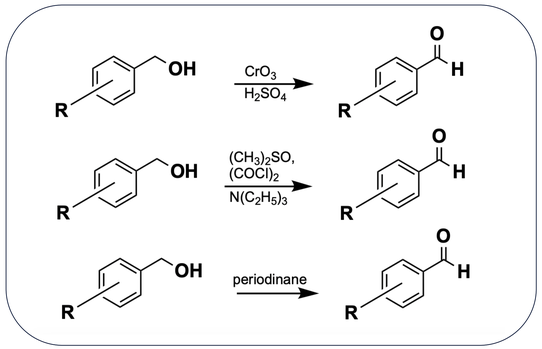

Figure 2. Traditional preparations of benzaldehyde using carcinogenic, toxic, and explosive reagents.[6]

OUR CLEANER, GREENER METHOD

Oxoammonium nitrate salt

- Our proposed method uses an oxoammonium salt with a nitrate anion as an oxidant.
- While this oxoammonium cation has been used previously, our lab introduced an additional nitrogen oxide regeneration cycle (Figure 3).[7]

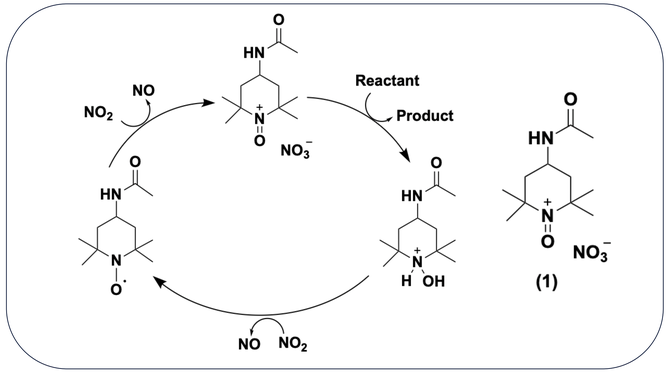

Figure 3. Catalytic recyclization of oxoammonium nitrate salt during oxidation.

Oxidation of Benzylamine to Benzaldehyde

- The nitrate salt (1) was used to oxidize benzylamine to benzaldehyde, using water as a solvent.
- The reaction mixture is stirred in a 10 mL reaction tube under microwave assisted heating.
- The benzaldehyde product is washed with water and diethyl ether to be isolated as a clear liquid.

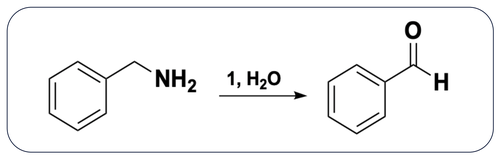

Figure 4. Green synthetic route to benzaldehyde from benzylamine.

RESULTS AND CONCLUSIONS

- We optimized the reaction conditions by systematically varying temperature, reaction time, and the amount of oxidant.
- Optimized conditions:

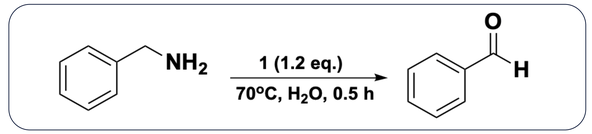

Figure 5. Reaction was performed in a sealed vessel using 0.5 mmol (1 eq.) of benzylamine.

- We see 100% conversion of our starting material (benzylamine) to our desired product (benzaldehyde).

ACKNOWLEDGEMENTS

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