Precision in organic synthesis: enhancing benzoic acid yield from benzaldehyde through reagent optimization

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Abstract : This study investigates the synthesis of benzoic acid from benzaldehyde, focusing on optimizing reaction conditions to maximize yield and purity. Various concentrations of sodium hydroxide (NaOH) and potassium permanganate ($KMnO_4$) were systematically evaluated under controlled laboratory conditions. Yields ranged from **7.37% to 27.8%,** with UV absorbance measurements confirming product purity. The optimal conditions were identified as 60% NaOH and 1.74 g $KMnO_4$, which produced the highest yield of **27.8%.** Conversely, lower concentrations led to decreased yields and purity. These findings highlight the critical role of reagent proportions in achieving efficient oxidation. This work provides a foundation for further improvements in the synthesis of benzoic acid, with potential applications in laboratory and industrial settings.

Keywords: Benzaldehyde, Benzoic Acid, Sodium Hydroxide, Potassium Permanganate, Oxidation, Organic Synthesis

Introduction

Benzoic acid, a versatile organic compound, is indispensable in industries such as food preservation, pharmaceuticals, and polymer manufacturing. Its efficient synthesis has garnered significant attention due to its widespread applicability and straightforward reaction mechanisms. The oxidation of benzaldehyde to benzoic acid, particularly using strong oxidizing agents, is one of the most widely studied reactions in organic chemistry. Among oxidizing agents, potassium permanganate ($KMnO_4$) has been a staple in both academic and industrial settings, owing to its strong oxidizing potential, stability, and ease of use [1,2]. The reaction is typically conducted in an alkaline medium, where sodium hydroxide (NaOH) enhances the reactivity by providing hydroxide ions necessary for the oxidation process [3]. However, the efficiency of this transformation is highly dependent on the proportions and concentrations of the reagents involved [4].While alternative oxidation methods, such as phase transfer catalysis (PTC)[5] and electrochemical oxidation[6], have emerged, the simplicity and effectiveness of KMnO4-based systems remain unmatched for benzoic acid synthesis. Recent studies have delved into optimizing reagent concentrations, reaction temperatures, and environmental conditions to improve both the yield and purity of the product [7,8]. Despite these advancements, challenges persist, particularly in minimizing side reactions and ensuring scalability for industrial applications[9].

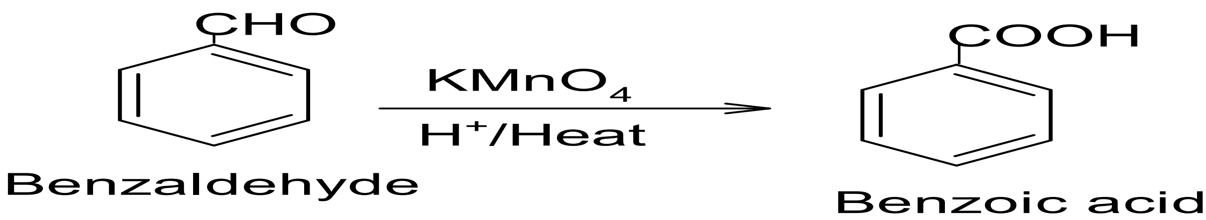
This study aims to systematically investigate the role of reagent proportions—specifically NaOH and KMnO4 concentrations—in the synthesis of benzoic acid. By combining yield analysis and UV spectroscopic purity assessment, this work seeks to establish optimal conditions for the reaction. Additionally, the study provides insights into avoiding conditions that may lead to inefficiencies or impurities, thereby contributing to the ongoing optimization efforts in organic synthesis[10].

Results and Discussion

The synthesis of benzoic acid from benzaldehyde was conducted using varying concentrations of NaOH and $KMnO_4$. The experimental results revealed significant correlations between reagent concentrations and reaction outcomes. **Effect of Sodium Hydroxide Concentration:** Higher concentrations of NaOH facilitated greater availability of hydroxide ions, which promoted deprotonation and subsequent oxidation of benzaldehyde. The highest yield of 27.8% was observed at 60% NaOH with 1.74 g KMnO4, while lower NaOH concentrations resulted in reduced yields. **Effect of Potassium Permanganate Amount:** Increasing KMnO4 quantities provided sufficient oxidizing power to drive the reaction. However, excessive KMnO4 concentrations led to minor side reactions, as indicated by slight deviations in UV absorbance values. This highlights the importance of balancing reagent proportions to achieve optimal results. **UV Spectroscopic Analysis:** UV absorbance measurements confirmed the purity of the synthesized benzoic acid. Most samples exhibited absorbance values closely matching the standard benzoic acid solution, with minor deviations observed at higher reagent concentrations.

Environmental factors such as temperature and humidity had minimal impact on the reaction outcomes, confirming the robustness of the synthesis under standard laboratory conditions. These findings underscore the critical role of reagent optimization in enhancing both yield and purity.

Chemical Reaction



Experimental Procedure

Materials and Methods:

Benzaldehyde: Fixed at 1.02 g per reaction. Potassium permanganate (KMnO4): 0.35 g, 0.58 g, and 1.74 g. Sodium hydroxide (NaOH): 20%, 30%, 40%, 50%, and 60% solutions. Distilled water: Used for recrystallization.

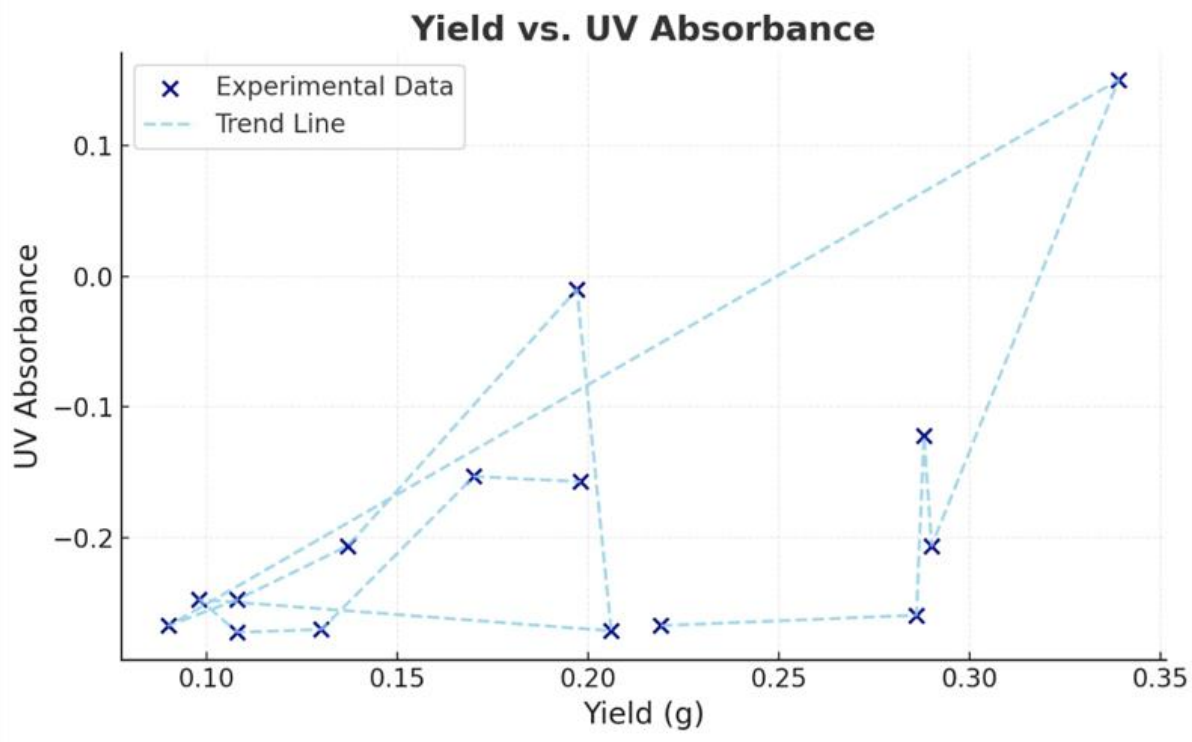
Methodology:

A reaction vessel was charged with 1.02 g of benzaldehyde and NaOH solution of a specific concentration. **(Table 1)** $KMnO_4$ was gradually added under constant stirring to ensure controlled oxidation. The reaction mixture was maintained at room temperature with periodic stirring. The reaction was quenched by adding distilled water, and the precipitated benzoic acid was filtered. Crude benzoic acid was recrystallized using distilled water to obtain a purified product. The mass of the purified product was measured, and the yield was calculated as a percentage of the theoretical yield. UV absorbance of the product was analysed using a UV-Vis spectrophotometer. **(Fig.1)**

Sr No.	Benzaldehyde (g)	$KMnO_4$ (g)	%NaOH	Benzoic Acid (g)	% Yield	UV Absorbance
1	1.02	1.74	20	0.219	18	-0.267
2	1.02	1.74	30	0.286	23.4	-0.259
3	1.02	1.74	40	0.288	23.6	-0.122
4	1.02	1.74	50	0.290	23.7	-0.206
5	1.02	1.74	60	0.339	27.8	0.150
6	1.02	0.58	20	0.090	7.37	-0.267
7	1.02	0.58	30	0.108	8.8	-0.247
8	1.02	0.58	40	0.137	11.22	-0.206
9	1.02	0.58	50	0.197	16.14	-0.010
10	1.02	0.58	60	0.206	16.9	-0.271
11	1.02	0.35	20	0.098	8.03	-0.247
12	1.02	0.35	30	0.108	8.85	-0.272

13	1.02	0.35	40	0.130	10.6	-0.270
14	1.02	0.35	50	0.170	13.9	-0.153
15	1.02	0.35	60	0.198	16.22	-0.157

Graph:



Conclusion

This study demonstrates that the optimal conditions for synthesizing benzoic acid from benzaldehyde involve using 60% NaOH and 1.74 g KMnO4, achieving a maximum yield of 27.8%. The purity of the product was confirmed through UV spectroscopic analysis. These findings emphasize the significance of reagent optimization in driving efficient oxidation reactions and achieving high-quality outcomes. Future research should explore alternative oxidizing agents, reaction conditions, and scalability to further improve yield and sustainability in benzoic acid synthesis.

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