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Optimization of the Synthesis Parameters of (E)-4-(Dimethylamino)-N-Benzylideneaniline

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Abstract. *Schiff bases containing azomethine functional groups continue to attract considerable interest due to their structural diversity and broad applicability in coordination chemistry, organic synthesis, and functional material design. In the present study, (E)-4-(dimethylamino)-N-benzylideneaniline was synthesized through the condensation reaction of 4-dimethylaminobenzaldehyde with aniline in ethanol medium under mild acidic conditions. The influence of major synthesis parameters, including reaction temperature, reaction time, and catalyst amount, on product yield and crystallization behavior was systematically investigated. The reaction progress was visually monitored through changes in solution color and crystal formation. Experimental results demonstrated that the synthesis efficiency strongly depended on reaction conditions. Moderate temperatures promoted effective azomethine bond formation, whereas excessive heating reduced product quality and yield. The optimal synthesis conditions were determined to be 50 °C reaction temperature, 35 minutes reaction time, and the addition of two drops of acetic acid catalyst. Under these conditions, the target Schiff base was obtained as an intense yellow crystalline compound with high yield. The study confirms that mild reaction conditions provide an efficient and experimentally simple approach for the synthesis of conjugated azomethine derivatives.*

Keywords: *schiff base, azomethine, condensation reaction, synthesis optimization, dimethylaminobenzaldehyde, aniline*

Introduction

Schiff bases represent an important class of organic compounds containing the azomethine (-CH=N) functional group formed by condensation reactions between primary amines and carbonyl compounds. Due to the presence of electron-rich nitrogen atoms and conjugated π-electron systems, these compounds have attracted continuous attention in coordination chemistry, catalysis, medicinal chemistry, optical materials, and analytical applications (Huseynova et al., 2025).

The structural and physicochemical properties of Schiff bases strongly depend on the nature of substituent groups attached to the aromatic system. Electron-donating substituents such as dimethylamino groups significantly influence electron delocalization within the molecule and affect the stability, color, and crystallization behavior of the resulting azomethine derivatives.

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Aromatic Schiff bases containing donor substituents are particularly interesting because of their extended conjugation systems and enhanced electronic interactions (Rajanna et al., 2025). Among substituted azomethine compounds, Schiff bases derived from 4-dimethylamino benzaldehyde have gained increasing attention because the dimethylamino group substantially modifies the electronic distribution of the aromatic framework (Waziri et al., 2023). The electron-releasing nature of this substituent increases electron density within the conjugated system and promotes stabilization of the imine functionality. Such electronic effects may alter molecular polarity, intermolecular interactions, and reactivity toward electrophilic or coordination processes (Fejfarova et al., 2010).

Structurally, these compounds generally adopt the thermodynamically favorable E-configuration around the azomethine bond (Awad et al., 2020). The spatial arrangement associated with the E-isomer contributes to molecular stability by reducing steric repulsion between aromatic fragments and improving π-conjugation throughout the molecular skeleton. Extended conjugation is also responsible for the intense coloration commonly observed in dimethylamino-substituted Schiff bases (Soliz et al., 2024).

In recent years, Schiff bases containing dimethylamino substituents have been investigated for a wide variety of applications. Numerous studies have demonstrated that such compounds and their metal complexes may exhibit antibacterial, antifungal, antioxidant, and anticancer activities (Ahmed et al., 2020). In many cases, coordination of Schiff bases with transition metal ions enhances biological efficiency due to modifications in lipophilicity, electronic structure, and metal-assisted transport processes (You et al., 2004).

Beyond medicinal applications, conjugated Schiff bases are also considered promising functional materials (Ali et al., 2022). Their ability to coordinate with metal ions enables their utilization in sensor technology, electrochemical systems, and corrosion inhibition studies. The presence of donor nitrogen atoms and aromatic π-systems facilitates adsorption on metallic surfaces and contributes to the formation of stable coordination environments (Trzesowska-Kruszynska, 2010). Additionally, intermolecular interactions such as π–π stacking and weak hydrogen bonding may influence crystal packing, solubility, and physicochemical stability (Khalaji et al., 2011).

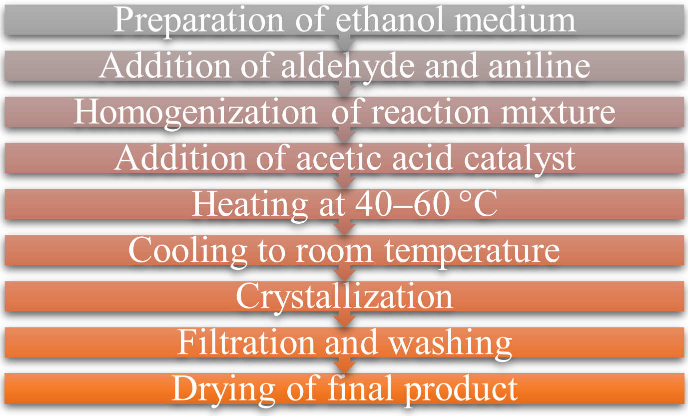
Despite the simplicity of Schiff base synthesis, optimization of experimental parameters remains critically important for obtaining products with high yield and desirable purity. Reaction temperature, catalyst concentration, solvent polarity, and reaction duration directly influence the rate of nucleophilic addition, dehydration efficiency, and subsequent crystallization behavior. Therefore, systematic evaluation of synthesis conditions is necessary for establishing reproducible and experimentally efficient synthetic methodologies (Ngoudjou et al., 2023).

In this study, (E)-4-(dimethylamino)-N-benzylideneaniline was synthesized from 4-dimethylaminobenzaldehyde and aniline in ethanol medium under mild acidic conditions. The effects of reaction temperature, reaction time, and catalyst amount on synthesis efficiency were comparatively investigated in order to determine the optimal experimental conditions for azomethine bond formation.

Materials and Methods

4-Dimethylaminobenzaldehyde, aniline, ethanol, and acetic acid were used without additional purification. All reagents were of analytical grade. The synthesis procedure was carried out using a magnetic stirrer, water bath, analytical balance, filtration apparatus, and drying oven.

General Synthesis Procedure



Initially, 10–15 ml of ethanol was introduced into a reaction flask. Equimolar amounts of 4-dimethylaminobenzaldehyde and aniline were then added to the solvent medium. The mixture was stirred until a homogeneous solution was obtained. Subsequently, 2–3 drops of acetic acid were added as a catalyst to accelerate the condensation process. The reaction mixture was heated in a water bath at temperatures ranging from 40 to 60 °C for 30–40 minutes under continuous stirring. During heating, gradual color changes were observed, indicating the formation of the azomethine linkage. After completion of the reaction, the mixture was cooled to room temperature. Formation of a crystalline precipitate was observed during the cooling stage. In cases where precipitation was incomplete, a small quantity of distilled water was added to facilitate crystallization.

The obtained solid product was separated by filtration, washed with cold ethanol, and dried at 50–60°C. The synthesis reaction proceeded according to the following equation:

$$(CH_3)_2N-C_6H_4-CHO + C_6H_5NH_2 \rightarrow (CH_3)_2N-C_6H_4-CH=N-C_6H_5 + H_2O$$

Optimization studies

The influence of three major synthesis parameters was investigated: Reaction temperature; Reaction time; Catalyst amount. The isolated product yield was calculated gravimetrically after drying.

Results

Effect of Reaction Temperature

The effect of temperature on product formation was investigated under identical reaction conditions.

Figure 1

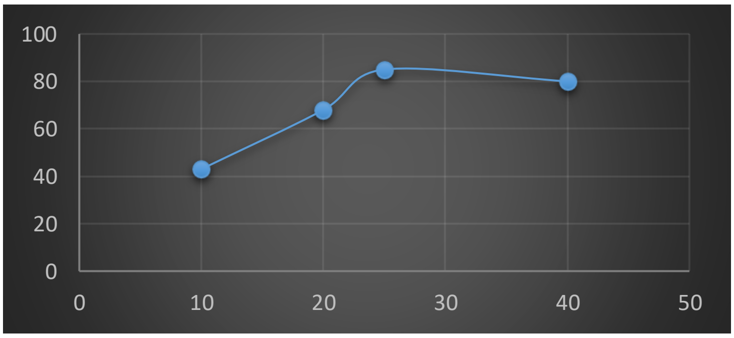
The process of obtaining a crystalline product

Temperature (°C)	Reaction time (min)	Yield (%)	Product appearance
30	35	56	Pale yellow crystals
40	35	72	Yellow crystals
50	35	85	Intense yellow crystals
60	35	80	Dark yellow crystals

The results indicate that increasing the temperature from 30 °C to 50 °C significantly improved product yield. However, further increase in temperature slightly reduced the efficiency of the synthesis.

Effect of Reaction Time

The influence of reaction duration on product formation was also evaluated. The highest yield was obtained after 35 minutes of heating.



Effect of Catalyst Amount

The influence of catalyst concentration on the synthesis efficiency of (E)-4-(dimethylamino)-N-benzylideneaniline was investigated using different amounts of acetic acid under identical reaction conditions. The experimental results demonstrated that catalyst quantity significantly affected the formation of the azomethine linkage and the overall product yield.

When one drop of acetic acid was used, the isolated yield of the product reached 61%, indicating that the catalytic activation of the carbonyl group was relatively limited under these conditions. Increasing the catalyst amount to two drops considerably improved the reaction efficiency and resulted in the highest yield of 84%. This improvement can be attributed to enhanced protonation of the carbonyl oxygen, which facilitated nucleophilic attack by aniline and accelerated imine formation.

However, further increase of the catalyst amount to five drops led to a decrease in product yield to 73%. Excessive acidic conditions likely affected the crystallization process and promoted partial side reactions, resulting in lower isolation efficiency of the Schiff base product. The obtained results indicate that moderate catalyst concentration provides the most favorable conditions for efficient synthesis of the target azomethine derivative.

Discussion

The obtained results demonstrate that synthesis efficiency is strongly dependent on reaction parameters. The condensation reaction between 4-dimethylaminobenzaldehyde and aniline proceeds through nucleophilic attack of the amine nitrogen on the carbonyl carbon atom, followed by dehydration and formation of the azomethine linkage. The dimethylamino substituent acts as an electron-donating group and increases electron density within the aromatic system. This electronic effect contributes to stabilization of the conjugated structure formed after condensation. As a result, the synthesized Schiff base exhibits intense coloration associated with extended π-electron delocalization (Hassan & Yusoff, 2019).

Temperature was found to be one of the most influential factors affecting product formation. At lower temperatures, insufficient molecular collisions slowed down the condensation process, resulting in lower yields. Moderate heating accelerated azomethine bond formation and improved crystallization efficiency. However, excessive heating likely promoted secondary processes and reduced product purity.

Reaction duration also affected the synthesis outcome. Short reaction periods did not allow complete conversion of reactants, whereas prolonged heating slightly decreased yield, probably due to partial decomposition or side reactions. Acetic acid played an important catalytic role by activating the carbonyl group toward nucleophilic attack. Nevertheless, excessive catalyst concentration negatively influenced crystal formation, leading to reduced isolated yields.

Overall, the experimental results confirmed that mild synthetic conditions can efficiently produce conjugated Schiff base derivatives with relatively high yields and simple experimental procedures.

Conclusion

(E)-4-(Dimethylamino)-N-benzylideneaniline was successfully synthesized through condensation of 4-dimethylaminobenzaldehyde with aniline in ethanol medium under acidic conditions. The influence of reaction temperature, reaction time, and catalyst amount on synthesis efficiency was systematically investigated. Optimal conditions were determined as 50 °C reaction temperature, 35 minutes reaction time, and two drops of acetic acid catalyst.

Under these conditions, the target Schiff base was obtained as an intense yellow crystalline product with high yield. The experimental findings demonstrated that careful optimization of reaction parameters significantly improves azomethine bond formation, crystallization efficiency, and overall synthetic performance.

The electronic influence of the dimethylamino substituent contributes to stabilization of the conjugated structure and may enhance the coordination ability and functional applicability of the synthesized compound. Owing to its conjugated molecular architecture and donor nitrogen center, the synthesized Schiff base may serve as a promising precursor for future investigations in coordination chemistry, functional materials, corrosion inhibition, and biologically active metal complexes.

Declaration of Competing Interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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