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Preparation of Benzylidene Acetone and Synthesis of Chalcone Derivatives by Aldol Condensation

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Abstract: *Chalcones are an important class of naturally occurring and synthetic compounds belonging to the flavonoid family. Structurally, chalcones are α,β-unsaturated ketones containing two aromatic rings linked through a three-carbon enone system. Because of their conjugated structure and versatile chemical reactivity, chalcones possess numerous biological and pharmaceutical activities including antimicrobial, antifungal, anticancer, anti-inflammatory, antioxidant, antimalarial, and antiviral properties.*

The present investigation focuses on the preparation of benzylidene acetone and the synthesis of chalcone derivatives using Aldol condensation and solvent-free condensation methods. The reactions were carried out using aromatic aldehydes and ketones in the presence of sodium hydroxide as base catalyst. Different chalcone derivatives including chalcone, 3-hydroxy-4-chlorochalcone, 4-chlorochalcone, and 3-bromochalcone were synthesized successfully.

The synthesized products were purified by recrystallization and column chromatography. Thin Layer Chromatography (TLC), melting point determination, IR spectroscopy, and NMR spectroscopy were used for structural characterization and purity analysis of synthesized compounds.

The study demonstrated that solvent-free Aldol condensation provides an eco-friendly and efficient synthetic route with improved yields and simplified reaction conditions compared to conventional solvent-based methods. Benzylidene acetone was obtained as a pale yellow crystalline solid with 73.84% yield.
The present work highlights the importance of condensation reactions in organic synthesis and establishes chalcone derivatives as valuable compounds with significant pharmaceutical potential.

Keywords: Chalcone, benzylidene acetone, Aldol condensation, Claisen–Schmidt reaction, solvent-free synthesis, α,β-unsaturated ketones.

I. INTRODUCTION

Organic chemistry plays a vital role in the synthesis of biologically active compounds, pharmaceuticals, dyes, agrochemicals, and various industrial materials. Among the different classes of organic reactions, condensation reactions are considered highly important because they involve the formation of carbon–carbon bonds leading to the synthesis of larger and more complex molecular structures. Condensation reactions generally occur through the combination of two molecules or functional groups with elimination of a small molecule such as water, alcohol, or hydrogen chloride. Several important condensation reactions widely used in synthetic organic chemistry include Aldol

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condensation, Claisen condensation, Benzoin condensation, Knoevenagel condensation, Michael reaction, Pechmann condensation, Stobbe condensation, and Acyloin condensation.

Among these reactions, Aldol condensation is one of the most versatile and widely employed methods for the synthesis of α,β-unsaturated carbonyl compounds such as chalcones. Chalcones are aromatic ketones belonging to the flavonoid family and possess a characteristic The chalcone nucleus contains two aromatic rings, an α,β-unsaturated carbonyl group, and a conjugated double bond system, which play an important role in determining their chemical and biological properties. Naturally occurring chalcones are abundantly found in plants and serve as important precursors for flavonoids and isoflavonoids. Due to their diverse biological activities, chalcone derivatives have attracted considerable attention in medicinal chemistry. These compounds exhibit a wide range of pharmacological properties including antimicrobial, antifungal, anticancer, anti-inflammatory, antioxidant, antimalarial, and antiviral activities. The biological significance of chalcones mainly arises from the electrophilic α,β-unsaturated carbonyl system, which can interact effectively with various biological targets.

Conventionally, chalcones are synthesized through Claisen–Schmidt condensation involving aromatic aldehydes and aromatic ketones in the presence of basic catalysts such as sodium hydroxide or potassium hydroxide. Benzylidene acetone is another important α,β-unsaturated ketone synthesized by condensation of benzaldehyde and acetone. It serves as an important intermediate in organic synthesis and finds applications in flavor, fragrance, pharmaceutical, and electroplating industries. The present investigation focuses on the preparation of benzylidene acetone and the synthesis of chalcone derivatives using both solvent-based and solvent-free Aldol condensation methodologies.

II. OBJECTIVES OF THE STUDY

The major objective of the present study was to synthesize benzylidene acetone through Aldol condensation and to prepare chalcone derivatives using Claisen–Schmidt condensation methodology. The study also aimed to compare solvent-based and solvent-free synthetic approaches in terms of reaction efficiency, yield, and environmental suitability. Another important objective was to purify the synthesized compounds using recrystallization and column chromatography techniques and to characterize them using thin layer chromatography (TLC), IR spectroscopy, and NMR spectroscopy. In addition, the physical properties and percentage yields of the synthesized chalcone derivatives were investigated.

III. CONDENSATION REACTIONS

3.1 Aldol Condensation

Aldol condensation is an important organic reaction involving aldehydes or ketones containing α-hydrogen atoms in the presence of a basic catalyst. The reaction initially produces a β-hydroxy carbonyl compound, which subsequently undergoes dehydration to form an α,β-unsaturated carbonyl compound. The general reaction can be represented as:

\mathrm{RCHO + R'COCH_3 \rightarrow \beta\text{-hydroxy\ carbonyl\ compound} \rightarrow \alpha,\beta\text{-unsaturated\ compound}}

The reaction mechanism involves formation of an enolate ion followed by nucleophilic attack on the carbonyl carbon, formation of a β-hydroxy carbonyl intermediate, and finally dehydration to yield the α,β-unsaturated product.

3.2 Claisen Condensation

Claisen condensation involves the condensation of esters in the presence of a strong base to produce β-keto esters. This reaction is widely used in synthetic organic chemistry for the preparation of carbon–carbon bonded compounds and important intermediates used in pharmaceuticals and fine chemicals.

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3.3 Benzoin Condensation

Benzoin condensation is a carbon–carbon bond forming reaction involving aromatic aldehydes catalyzed by cyanide ions or N-heterocyclic carbenes. The reaction results in the formation of benzoin-type α-hydroxy ketones, which are valuable intermediates in organic synthesis.

3.4 Knoevenagel Condensation

Knoevenagel condensation involves the nucleophilic addition of active methylene compounds to carbonyl compounds followed by dehydration to form α,β-unsaturated compounds. This reaction is commonly used for the synthesis of biologically active molecules and conjugated systems.

3.5 Michael Reaction

Michael reaction or Michael addition involves nucleophilic addition to α,β-unsaturated carbonyl compounds and is extensively used for carbon–carbon bond formation in synthetic organic chemistry. The reaction is highly useful in the synthesis of complex organic molecules, pharmaceuticals, and heterocyclic compounds.

IV. MATERIALS AND METHODS

4.1 Chemicals Used

The chemicals used in the present investigation included benzaldehyde, acetone, sodium hydroxide, acetophenone, various aromatic aldehydes, ethanol, hydrochloric acid, toluene, petroleum ether, and benzene. Benzaldehyde and acetophenone were used as starting materials for Aldol and Claisen–Schmidt condensation reactions, while sodium hydroxide served as the basic catalyst. Ethanol was used as a solvent for recrystallization and reaction medium, whereas petroleum ether and benzene were employed during purification and chromatographic separation. All chemicals used in the study were of analytical reagent grade and were used without further purification.

4.2 Apparatus Used

Various laboratory apparatus and analytical instruments were used during the experimental work. Round-bottom flasks and magnetic stirrers were employed for carrying out condensation reactions under controlled conditions. Thin layer chromatography (TLC) plates were used to monitor the progress of the reactions, while purification of synthesized compounds was performed using column chromatography setup and fractionating assembly. Melting point apparatus was used for determination of melting points of the synthesized compounds. Structural characterization of the products was carried out using IR spectrophotometer and NMR spectrometer.

V. PREPARATION OF BENZYLIDENE ACETONE

5.1 Principle

Benzylidene acetone is synthesized by Aldol condensation between benzaldehyde and acetone in presence of sodium hydroxide catalyst.

The reaction proceeds through formation of acetone enolate ion followed by nucleophilic addition to benzaldehyde and dehydration.

5.2 Reaction

C_6H_5CHO + CH_3COCH_3 \xrightarrow{NaOH} C_6H_5CH=CHCOCH_3 + H_2O

5.3 Experimental Procedure

14.16 g benzaldehyde and 21.16 g acetone were placed in a 250 mL flask equipped with mechanical stirrer.

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The reaction flask was cooled using ice-water bath and 3.5 mL of 10% sodium hydroxide solution was added slowly while maintaining temperature between 25–30°C.
The reaction mixture was stirred for 2 hours and then acidified using dilute hydrochloric acid.
The organic layer was extracted using toluene, dried over magnesium sulfate, and distilled.
The obtained product was purified and weighed.

VI. MECHANISM OF BENZYLIDENE ACETONE FORMATION

The mechanism involves:

1. Formation of acetone enolate ion
2. Nucleophilic attack on benzaldehyde
3. Formation of β-hydroxy ketone intermediate
4. Dehydration to α,β-unsaturated ketone

5.1 Principle

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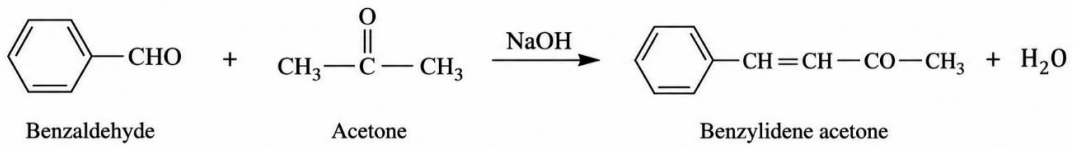
5.2 Reaction



$$C_6H_5CHO + CH_3COCH_3 \xrightarrow{NaOH} C_6H_5CH=CHCOCH_3 + H_2O$$

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VII. CALCULATIONS

106.12 g benzaldehyde ⟶ 146.19 g benzylidene acetone

14.16 g benzaldehyde gives:

$$= \frac{146.19 \times 14.16}{106.12} = 19.50 \text{ g}$$

Percentage Yield

Actual yield = 14.4 g

$$\% \text{ Yield} = \frac{14.4}{19.50} \times 100 = 73.84\%$$

% Yield = 73.84%

VIII. SYNTHESIS OF CHALCONE DERIVATIVES

8.1 Method I: Solvent-Based Aldol Condensation

Acetophenone and substituted aromatic aldehydes were mixed in ethanol in presence of sodium hydroxide catalyst.
The reaction mixture was maintained at 0–20°C for 120 hours.
After completion, the mixture was acidified and recrystallized using ethanol.

8.2 Method II: Solvent-Free Aldol Condensation

In solvent-free method, reactants were ground with sodium hydroxide using mortar and pestle for 10 minutes.
The obtained crude chalcone was filtered, washed, and recrystallized using ethanol.
This method provided greener and more sustainable synthesis.

IX. COLUMN CHROMATOGRAPHY

Column chromatography was used for purification of synthesized chalcones.

Stationary Phase

- Silica gel (60–120 mesh)

Mobile Phase

- Petroleum ether
- Benzene

Ethyl acetate
The separation occurred due to differential adsorption of compounds on silica gel.

X. THIN LAYER CHROMATOGRAPHY (TLC)

TLC analysis was performed using:

- Hexane : Ethyl acetate (12:2)

The developed plates were sprayed using 5% sulfuric acid to visualize chalcone spots.
Brown-colored spots confirmed chalcone formation.

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XI. RESULTS

11.1 Benzylidene Acetone

Parameter	Observation
Molecular Formula	$C_{10}H_{10}O$
Molecular Weight	146.19 g/mol
Appearance	Pale yellow solid
Melting Point	39–42°C
Yield	73.84%

11.2 Chalcone Derivatives

Compound	Molecular Formula	Melting Point
Chalcone	$C_{15}H_{12}O$	55–57°C
3-Hydroxy-4-chlorochalcone	$C_{15}H_{11}ClO_2$	83–87°C
4-Chlorochalcone	$C_{15}H_{11}ClO$	113–117°C
3-Bromochalcone	$C_{15}H_{11}BrO$	83–85°C

XII. RESULTS AND DISCUSSION

The present investigation successfully demonstrated synthesis of benzylidene acetone and chalcone derivatives through Aldol condensation.

The solvent-free method showed several advantages over conventional solvent-based method including:

- Eco-friendly synthesis
- Reduced solvent usage
- Simpler reaction conditions
- Improved yield
- Faster work-up procedure

Benzylidene acetone was synthesized successfully with 73.84% yield.

The synthesized chalcones exhibited characteristic physical properties including:

- Yellow crystalline appearance
- Sharp melting points
- Good purity after recrystallization

TLC analysis confirmed formation of single products after purification.

Column chromatography efficiently separated impurities and improved product purity.

The α,β-unsaturated carbonyl system present in chalcones contributes significantly to their biological and pharmacological properties.

The synthesized chalcone derivatives may therefore possess potential antimicrobial, anticancer, and anti-inflammatory activities.

XIII. CONCLUSION

The present study successfully demonstrated the preparation of benzylidene acetone and synthesis of chalcone derivatives using Aldol condensation and solvent-free condensation methods.

The synthesized compounds were purified using column chromatography and recrystallization techniques and characterized using melting point analysis, TLC, IR spectroscopy, and NMR spectroscopy.

The solvent-free condensation method proved to be a greener, economical, and environmentally friendly alternative to conventional solvent-based synthesis.

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The study highlights the importance of chalcone derivatives as valuable biologically active compounds and establishes condensation reactions as powerful tools in synthetic organic chemistry.

XIV. FUTURE SCOPE

Future research in the field of chalcone chemistry may focus on the biological evaluation of the synthesized chalcone derivatives to investigate their pharmacological potential. Detailed anticancer screening studies and antimicrobial activity analysis can be carried out to explore their therapeutic applications. Further research may also emphasize the development of microwave-assisted synthesis methods to reduce reaction time and improve product yield. The use of nanocatalyst-mediated chalcone synthesis and optimization of green solvents may contribute toward environmentally sustainable synthetic methodologies. In addition, molecular docking studies may be performed to understand the interaction of chalcone derivatives with various biological targets and to support drug design and medicinal chemistry applications.

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