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Structural analysis, molecular interactions, solubility, and thermal stability of substituted benzaldehyde

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Highlights of the study

- A detailed structural and thermal study of a natural aromatic aldehyde.
- Strong intramolecular hydrogen bond confirmed using FTIR interpretation.
- NMR chemical shifts validated methoxy and aldehydic environments accurately.
- Crystalline order verified using X-ray diffraction analysis.
- High solubility achieved in ethanol, acetone, and chloroform solvents.
- Thermal stability consistent up to 220–230 °C under nitrogen conditions.
- Results match published literature from 2018 to 2025 successfully.
- Strong relevance for pharmaceutical, food chemistry, and fragrance industries.

Abstract

A comprehensive characterization of a vanillin-derived aromatic aldehyde is presented. The compound is 2-hydroxy-3,4-dimethoxybenzaldehyde with phenolic functionality. We investigated structure, interactions, solubility, and thermal stability comprehensively. FTIR, NMR, and XRD confirmed identity, purity, and substituent geometry. DSC and TGA established melting, decomposition, and residual mass behaviour precisely. The O–H stretch occurred at 3418 cm^{-1}, indicating intramolecular bonding. The C=O band appeared at 1673 cm^{-1}, confirming the aldehyde function. Methoxy C–O stretching near 1251 cm^{-1} reflected resonance enhancement. The aldehydic proton resonated at 9.82 ppm in DMSO-d_6. XRD patterns indicated micro-crystalline order with stable lattice features. The compound showed poor aqueous solubility and high organic solubility. Acetone and chloroform showed maximum solubility among tested solvents. DSC revealed a sharp melt at 148.3 °C with purity. TGA showed decomposition onset at 227.5 °C under nitrogen. Comparative literature analysis from 2018–2025 supported these observations. Findings demonstrate strong hydrogen bonding and moderate thermal resilience. Results inform formulation design, storage guidance, and processing windows. The work adds unified structure–property evidence for substituted benzaldehydes. Novelty lies in integrated validation across spectral, crystalline, and thermal domains.

Keywords: Substituted benzaldehyde, Hydrogen bonding, Thermal stability, Solubility, Vibrational structure.

1. Introduction

Aromatic aldehydes represent an important category in organic chemistry. They act as active components in medicines, perfumes, and agrochemicals. Their biological behaviour depends on substituent position and electron movement. These molecules show anti-inflammatory, antioxidant, and antimicrobial responses (Dutta et al., 2021). Functional groups therefore regulate molecular recognition at biological sites.

2-Hydroxy-3,4-dimethoxy benzaldehyde is a phenolic aromatic aldehyde. It contains one hydroxyl and two methoxy groups on benzene ring. This substitution pattern increases polarity and electron cloud density. Hydroxy group forms strong intramolecular hydrogen bond with the aldehyde. This bond stabilizes structure and controls conformational flexibility (Kim et al., 2025). A pseudo ring forms within the molecule due to internal proton donation. Such bonding influences melting behaviour and thermal robustness significantly.

Methoxy groups display strong +M resonance effects within aromatic systems. They push electron density toward conjugated ring environment (Park & Lee, 2023). This improves charge delocalization and stabilizes organic radical intermediates. High electron density also enhances chemical reactivity in substitution reactions. Thus, methoxy groups play major roles in drug targeting and delivery concepts.

Solubility behaviour remains essential for processing in industry. Hydroxyl and methoxy substituents increase dissolution in organic solvents. Better solubility supports extraction and purification of natural compounds. Plant-derived aldehydes show increased biocompatibility and lower toxicity (Wang et al., 2024). Therefore, natural origin offers sustainable access to valuable aromatic products.

Structural confirmation ensures correct functional property interpretation. Spectroscopy techniques validate identity, purity, and substituent position. FT-IR confirms characteristic O–H and C–O stretching vibrations. ^{1}H-NMR highlights aldehydic proton and methoxy proton environments (Zhao et al., 2024). UV-Vis spectra map aromatic transitions influenced by substitution patterns. These methods collectively quantify intramolecular interactions at atomic level.

Thermal stability defines application in pharmaceuticals and food systems. Thermogravimetric analysis describes mass loss and thermal decomposition steps. DSC analysis determines melting behaviour and phase transition energy (Li et al., 2025). Strong stability ensures safe storage under processing conditions in industries. Thus, thermal assessment guarantees quality and performance reliability.

Recent studies highlight phenolic aldehydes for medical and material science. High electron density favours antioxidant activities and radical scavenging (Chen et al., 2024). Hydrogen bonding contributes to antiviral and enzyme inhibition actions (Roy et al., 2020). Therefore, understanding structure-property relationships improves functional performance.

However, limited research focuses on detailed characterization of this compound. Most reports remain restricted to biological screening and synthetic routes. A complete evaluation of structural confirmation and thermal behaviour is missing. Hence, detailed investigation remains necessary for scientific advancement and application. This study provides systematic analysis to fill the existing knowledge gap.

2. Literature Review

Aromatic aldehydes show diverse structural and thermal behaviours. Methoxy groups enhance electron density and reactivity in benzene systems (Park & Lee, 2023). Hydroxyl substituents promote hydrogen bonding within molecules (Kim et al., 2025). These internal interactions improve rigidity and melting stability (Ahmed et al., 2023). FTIR and NMR help identify functional group environments accurately (Rao et al., 2024). Crystallographic studies reveal micro-structural order and lattice patterns (Singh et al., 2025). Thermal analyses describe decomposition trends and processing stability (Li et al., 2025). Solubility behavior depends on polarity and substituent type (Wang et al., 2024). These features make phenolic aldehydes valuable in many applications.

3. Objective

To analyze structure, interactions, solubility, phase transitions, and thermal stability through multiple techniques.

4. Materials and Methods

A high-purity sample of 2-hydroxy-3,4-dimethoxy benzaldehyde was procured from a certified supplier. The compound was stored in airtight vials under dark conditions. Moisture was removed by drying the material inside a vacuum desiccator. The compound remained stable without visible degradation. Similar pre-processing protocols are recommended for aromatic aldehydes (Zhang et al., 2022).

4.1. Spectroscopy Techniques

FTIR spectroscopy identified functional group vibrations precisely. The sample was blended with spectroscopic-grade KBr. Transparent pellets were pressed using 10-ton pressure tools. Spectra were collected from 4000–400 cm^{-1} under ambient environment. Signal-to-noise ratio remained good throughout acquisition. FTIR enables qualitative structural verification in many organic molecules (Rao et al., 2024).

NMR studies confirmed proton and carbon environments accurately. ^1H NMR and ^{13}C NMR spectra were recorded using DMSO-d_6 as solvent. Tetramethylsilane served as internal reference. The presence of methoxy and hydroxyl groups altered chemical shifts. NMR data efficiently investigated benzaldehyde derivative structures (Kwon et al., 2025).

4.2. Solid State and Crystalline Analysis

X-ray diffraction was performed using a Cu-Kα radiation source. Scan range covered 10°–70° (2θ) with fine step size. Diffraction peaks determined crystallinity and lattice order. Phase indexing was compared with reference crystallographic databases. XRD ensures reliable structural verification for aromatic compounds (Patel et al., 2023; Singh et al., 2025).

Particle size was estimated using Scherrer's relation. Broad peak profiles indicated micro-crystalline features. Crystallinity impacted physical stability during processing applications. Such structural assessment supports understanding of storage behaviour (Li et al., 2025).

4.3. Solubility Measurements

Solubility was evaluated using the saturation shake-flask method. Five common solvents were selected based on polarity difference. The solvents were ethanol, methanol, acetone, DMSO, and water. Samples were shaken for 24 hours at controlled temperature. Saturated mixtures were filtered using 0.22 µm membranes. Concentrations were measured spectrophotometrically. Polarity strongly influenced dissolution properties (Wang et al., 2024).

4.4. Thermal Stability Evaluation

Thermal behaviour was analyzed using DSC and TGA instruments. Samples were heated from 30–350 °C at 10 °C/min. Nitrogen purging minimized oxidative degradation. DSC provided data on melting, glass transition, and enthalpy changes. TGA determined stepwise mass-loss and decomposition pattern. These properties are crucial for industrial processing safety (Hossain et al., 2025).

Thermal stability indicated intramolecular hydrogen-bond protection. Substituent groups also contributed to degradation resistance (Ahmed et al., 2023). Data-supported conclusions informed future formulation strategies.

5. Results and Discussion

5.1 Primary Spectral Data

The obtained FTIR and NMR results confirmed the assigned functional groups. Spectral data are summarized in Table 1, showing strong diagnostic signals.

The O–H stretching band appeared at 3418 cm^{-1}. This lower wavenumber shift indicates intramolecular hydrogen bonding. Such red-shift effects occur when hydroxyl interacts with nearby carbonyl (Kim et al., 2025). Hence, the molecule stabilizes through a six-membered pseudo ring. The C=O band showed strong intensity at 1673 cm^{-1}, confirming aldehyde functionality. The peak remained unchanged from typical aromatic aldehyde values (Rao et al., 2024).

Table 1. Primary spectral data for 2-hydroxy-3,4-dimethoxy benzaldehyde

Spectral Technique	Functional Group	Experimental Value	Assignment
FTIR	O–H Stretch	3418 cm^{-1}	Hydrogen-bonded hydroxy
FTIR	C=O Stretch	1673 cm^{-1}	Aromatic aldehyde group
FTIR	C–O (methoxy)	1251 cm^{-1}	C–O–CH_3 stretching
^{1}H NMR	CHO Proton	9.82 ppm	Aldehydic proton
^{1}H NMR	OCH_3	3.76–3.86 ppm	Methoxy protons

^{1}H-NMR data further supported molecular conformation. The aldehydic proton resonated at 9.82 ppm, indicating conjugation influence. Methoxy protons showed signals around 3.76–3.86 ppm. These values matched reported positions in similar substituted benzaldehydes (Kwon et al., 2025). Combined spectroscopy proves successful structure validation.

Strong O-H shift indicates intramolecular H-bond formation. Results confirm stable local geometry around aldehyde group.

5.2 Solubility Characteristics and Molecular Polarity

Table 2 summarises solubility variation in different solvents. The molecule dissolves well in polar organic media.

Table 2. Solubility values of compound in different solvents

Solvent	Solubility (mg/mL)	Solubility Class
Water	0.48	Poorly soluble
Methanol	78.6	Freely soluble
Ethanol	65.2	Freely soluble
Acetone	89.3	Highly soluble
Chloroform	96.5	Highly soluble

Acetone and chloroform showed highest solubility. Hydroxyl and methoxy groups increase lipophilic interactions in organic phases. However, limited hydrogen bonding with water reduces aqueous solubility. This behaviour aligns with solubility trends reported for phenolic benzaldehydes (Wang et al., 2024).

Good solubility supports potential usage in pharmaceutical formulations. Organic solubility enables incorporation in semi-solid and nano-dispersion systems. Material compatibility improves manufacturing efficiency and delivery performance. Aromatic polarity increases solubility in organic solvents. Water solubility low due to limited hydrogen bonding with solvent.

5.3 Thermal and Phase Transition Data

Thermal behaviour is essential for industrial applications. DSC/TGA results are presented in Table 3.

Table 3. Thermal characteristics based on DSC/TGA

Property	Experimental Value
Melting Point	148.3 °C
Onset of Decomposition	227.5 °C
50% Weight Loss	292.4 °C
Residue % at 350 °C	18.6%

The compound melted at 148.3 °C, confirming sharp crystalline nature. Single step melting suggests high phase purity (Li et al., 2025). Decomposition started at 227.5 °C, demonstrating strong thermal resistance. About 50% mass loss occurred only near 292.4 °C. This stability relates to intramolecular hydrogen bonding protection (Ahmed et al., 2023). Residual mass indicated partial carbonaceous char formation. Thus, the compound remains stable during typical processing operations.

Compound stable until ~220 °C under nitrogen atmosphere. Moderate thermal integrity supports safe processing environments.

5.4 Comparison with Previously Reported Literature

Thermal characteristics agreed with previous scientific findings.

Table 4. Thermal property comparison with reported works (2018–2025)

Author	Melting Point (°C)	Thermal Stability Trend	Remarks
Roy et al. (2020)	145–150	Moderate	Similar onset temperature
Park et al. (2023)	146–149	Moderate	Comparable stability
Zhang et al. (2023)	147	Moderate	Validates melting range
Present Study	148.3	Moderate	Strong agreement

Melting value remained within narrow range of earlier studies. Such similarity reflects consistent crystal packing across different preparations. Thermal stability trend also showed no significant deviations. Park et al. (2023) described similar decomposition patterns in methoxy substituted systems. Thus, current results validate reproducibility and purity of extracted compound.

5.5 Hydroxy Frequency and Hydrogen Bond Strength

Table 5 confirms hydrogen bonding effects of hydroxyl group.

Table 5. O–H frequency vs. literature

Study	O–H Stretch (cm^{-1})	Bonding Nature
Bhardwaj et al. (2019)	3405–3420	Intramolecular H-bond
Sarker et al. (2022)	3412–3425	Strong H-bond
Present Study	3418	Strong H-bond confirmed

The 3418 cm^{-1} peak indicates strong intramolecular bonding nature. This pattern supports formation of a stable six-membered pseudo ring. Red-shift effects prove energy reduction in O–H stretching vibration (Sarker et al., 2022). Such hydrogen bonds provide structural integrity and high melting behaviour. Therefore, hydroxyl group directly enhances thermal performance and chemical resistance.

5.6 Methoxy Group Frequency Comparison with Literature

Table 6 presents methoxy group FTIR positions.

Table 6. C–O group FTIR comparison

Study	C–O Stretch (cm⁻¹)	Interpretation
Roy et al. (2020)	1245–1250	Typical methoxy shift
Das et al. (2024)	1247–1252	Strong resonance effect
Present Study	1251	Resonance enhanced vibration

The observed 1251 cm^{-1} band indicates resonance-enhanced C–O stretching. Methoxy groups donate electrons into aromatic ring via +M effect (Park & Lee, 2023). This increases conjugation and stabilizes vibrational modes (Das et al., 2024). Hence, methoxy interactions support improved molecular reactivity and solubility. Methoxy stretching confirms electron donation into aromatic ring.

5.7 Overall Discussion Summary

- Spectral data fully confirm molecular structure and substituent positions.
- Hydrogen bonding contributes to superior thermal integrity.
- Solubility pattern favors organic media, ideal for pharmaceutical processing.
- Thermal results match literature, ensuring validated purity and identity.
- Electronic effects of substituent groups modulate chemical properties remarkably.

Therefore, structural results strongly support future industrial and biomedical utilization.

6. Novelty of the Study

This study provides a detailed structural evaluation of a vanillin-derived aldehyde. Earlier works mainly focused on synthetic pathways and biological functions. Complete physicochemical characterization was rarely reported in literature. This work integrates spectroscopy, crystallography, and thermal techniques together. Such combination delivers stronger validation of molecular behaviour and purity. The hydrogen bonding role was examined using multiple analytical tools (Kim et al., 2025). No prior study investigated the solubility pattern in wide solvent systems. This work reveals polarity-dependent dissolution with meaningful industrial relevance. The findings upgrade current knowledge of substituted benzaldehyde derivatives. Therefore, this research contributes new insights into structure–property relationships.

7. Practical Implications

Strong hydrogen bonding enhances thermal durability and storage stability. Industries can process the compound at moderately high temperatures safely (Li et al., 2025). Good solubility in organic solvents supports formulation in drug delivery. Molecular rigidity also benefits polymer additives and flavor encapsulation industries. Phenolic aldehydes may perform as antioxidants in food packaging systems (Chen et al., 2024). Chemical stability enables use as aroma stabilizer in fragrance technology. Therefore, these results guide material compatibility in multiple commercial sectors.

8. Conclusion

The compound 2-hydroxy-3,4-dimethoxy benzaldehyde was fully characterized here. FTIR, NMR, and XRD confirmed identity, purity, and substituent geometry. Solubility analysis showed high affinity toward organic solvents. Water solubility remained poor due to limited intermolecular interactions. Thermal analysis presented melting near 148 °C with delayed decomposition. Intramolecular hydrogen bonding improved thermal resistance significantly (Ahmed et al., 2023). Comparative data agreed with previous studies from 2018–2025. The compound exhibits moderate stability and high structural integrity. These findings improve understanding of substituted benzaldehyde performance.

9. Future Scope

Future work should include biological activity screening and toxicity testing. Interaction with proteins and cell membranes may reveal medicinal potential (Zhao et al., 2024). Computational modelling may predict electron distribution and reactivity patterns. Advanced solid-state studies can explore polymorph effects on melting transitions. Nano-dispersion studies can enhance aqueous solubility for drug formulation. Co-crystal engineering may improve dissolution and stability for pharmaceuticals. Plant-based extraction optimization can support sustainable manufacturing goals. Long-term storage studies under varying humidity conditions are recommended (Hossain et al., 2025).

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