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INVESTIGATION OF INFRARED SPECTROSCOPY AND RAMAN SPECTROSCOPY FOR FUNCTIONAL GROUP IDENTIFICATION AND STRUCTURAL CONFIRMATION OF TRI-SUBSTITUTED BENZALDEHYDE

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ABSTRACT

The structural characterization of substituted aromatic aldehydes is of considerable importance in organic, pharmaceutical, and analytical chemistry because of their widespread application as synthetic intermediates and biologically relevant molecules. In the present study, a detailed vibrational spectroscopic analysis of 2-hydroxy-3,4-dimethoxybenzaldehyde was carried out using the complementary techniques of infrared (IR) and Raman spectroscopy. The selected compound contains multiple functional groups, including hydroxyl (–OH), aldehyde (–CHO), and methoxy (–OCH_3) substituents, making it an ideal model for investigating substituent effects and vibrational interactions within an aromatic system. Infrared spectroscopy was utilized to identify characteristic absorption bands corresponding to carbonyl stretching, hydroxyl vibrations, methoxy C–O stretching, and fingerprint region features associated with aromatic substitution. Raman spectroscopy provided additional structural information through the detection of aromatic ring skeletal vibrations, ring-breathing modes, and other vibrational bands that were weak or inactive in the IR spectrum. The combined interpretation of IR and Raman spectra significantly improved the accuracy of vibrational band assignments and enabled a more comprehensive understanding of the molecular structure. The findings demonstrate that integrated IR–Raman spectroscopy is a reliable and efficient approach for the characterization of structurally complex tri-substituted benzaldehydes. The spectral assignments generated in this study may be valuable for organic synthesis verification, compound screening, and the development of spectral reference databases. Furthermore, the study emphasizes the future potential of combining experimental spectroscopy with computational modeling and machine learning tools for advanced structural analysis.

KEYWORDS: 2-Hydroxy-3,4-dimethoxybenzaldehyde; Infrared spectroscopy; Raman spectroscopy; Vibrational analysis; Aromatic aldehydes; Spectral characterization; Functional group assignment.

1. INTRODUCTION

Spectroscopic techniques play a fundamental role in organic chemistry, particularly in the elucidation and confirmation of molecular structures (Silverstein et al., 2016). These analytical methods offer rapid, reliable, and non-destructive identification of functional groups present in organic compounds (Banwell, 1966). Among the available spectroscopic approaches, vibrational spectroscopy is especially valuable for the characterization of substituted aromatic molecules due to

its sensitivity toward structural variations within aromatic frameworks (Schrader, 1995).

Infrared (IR) spectroscopy is based on the absorption of infrared radiation resulting from molecular vibrations that involve changes in dipole moment (Atkins & de Paula, 2002). Each functional group exhibits characteristic absorption frequencies within the infrared region, allowing their identification through distinct spectral bands (Banwell, 1966). Consequently, IR spectra provide important qualitative information regarding molecular structure and functional group composition (Silverstein et al., 2016).

Raman spectroscopy offers complementary structural information to that obtained from IR spectroscopy. This technique is based on the inelastic scattering of light, arising from changes in molecular polarizability during vibrational motion (Albrecht, 1961). Therefore, Raman spectroscopy is particularly useful for evaluating the symmetry properties of vibrational modes (Schrader, 1995). In many cases, vibrational modes that are weak or inactive in the IR spectrum appear strongly in Raman spectra, making the two techniques highly complementary for comprehensive molecular characterization (Banwell & McCash, 1994).

1.1 Infrared and Raman Spectroscopy Complementarity

The combined application of infrared (IR) and Raman spectroscopy significantly enhances the reliability of vibrational band assignments (Schrader, 1995). Since the two techniques are governed by different selection rules, spectral bands that may overlap or remain ambiguous in one method can often be clearly resolved in the other (Banwell & McCash, 1994). This complementary relationship minimizes misinterpretation and improves spectral accuracy, particularly in the analysis of structurally complex compounds such as multiphenolic systems (Silverstein et al., 2016).

IR spectroscopy is especially effective for identifying polar functional groups, owing to its sensitivity toward vibrations involving changes in dipole moment, as reported by Banwell (1966). In contrast, Raman spectroscopy is more responsive to non-polar vibrations and is particularly useful for investigating aromatic ring skeletal vibrations and ring-breathing modes (Schrader, 1995).

Therefore, the combined use of IR and Raman spectroscopy provides a more comprehensive understanding of molecular vibrational behavior. By integrating the strengths of both techniques, detailed structural information regarding functional groups as well as the molecular framework can be obtained, enabling complete vibrational characterization of organic compounds (Silverstein et al., 2016).

1.2 Vibrational Features of Aromatic Aldehydes

Aromatic aldehydes exhibit characteristic vibrational features that make them readily identifiable by spectroscopic techniques. One of the most important diagnostic absorptions is the carbonyl (C=O) stretching vibration, which appears as a prominent band in the infrared spectrum (Silverstein et al., 2016). In conjugated aromatic aldehydes, resonance interaction between the aldehyde group and the aromatic ring reduces the bond order of the carbonyl group, resulting in a shift of the C=O stretching frequency to lower wavenumbers (Badger, 1934).

In addition to the carbonyl absorption, aromatic aldehydes display weak but recognizable aldehydic C–H stretching vibrations, which serve as useful confirmatory signals in spectral analysis (Banwell, 1966). These characteristic bands contribute to the identification of the aldehyde functional group when interpreted together with the carbonyl stretching band.

The fingerprint region of the spectrum is typically dominated by aromatic ring vibrations, including C–C skeletal stretching and C–H bending modes (Schrader, 1995). Raman spectroscopy is particularly effective in detecting aromatic ring-breathing vibrations, which provide valuable information regarding the substitution pattern of the aromatic nucleus. These vibrations can be used to confirm the position and nature of substituents attached to the ring (Schrader, 1995).

Furthermore, the frequency and intensity of vibrational bands are strongly influenced by substituent effects such as electron-donating or electron-withdrawing interactions. These effects alter the electronic distribution within the aromatic system and consequently modify the vibrational behavior of the molecule (Badger, 1934). Thus, vibrational spectroscopy serves as a powerful tool for the structural characterization of aromatic aldehydes.

1.3 Influence of Phenolic and Methoxy Substitution

Phenolic and methoxy substituents exert a significant influence on the vibrational spectra of aromatic compounds through electronic effects and intermolecular interactions. Phenolic hydroxyl groups typically exhibit broad and intense O–H stretching bands in the infrared spectrum due to hydrogen bonding. The extent of broadening, band position, and intensity is strongly affected by both intermolecular and intramolecular hydrogen-bonding interactions, as well as by the nature and position of neighboring substituents (Badger, 1934; Silverstein et al., 2016).

Methoxy substituents contribute characteristic C–O stretching vibrations, which generally appear as strong and distinct absorption bands in the infrared region (Banwell, 1966). These bands are highly useful for confirming the presence of methoxy functionalities in substituted aromatic compounds. In addition, the methyl group attached to the methoxy moiety gives rise to C–H

bending and deformation vibrations, which may be prominently observed in Raman spectra (Schrader, 1995).

Electron-donating substituents such as hydroxyl and methoxy groups also alter the electron density of the aromatic ring through resonance effects. These changes influence vibrational coupling within the aromatic system, leading to shifts in band frequencies and variations in spectral intensities (Badger, 1934). Consequently, the presence and position of phenolic and methoxy groups play a crucial role in determining the vibrational behavior and spectroscopic characteristics of substituted aromatic molecules.

1.4 Structural Complexity in Tri-Substituted Benzaldehydes

Tri-substituted benzaldehydes exhibit considerable vibrational complexity because the presence, nature, and relative positions of multiple substituents strongly influence band frequencies, intensities, and splitting patterns. Interactions among substituents alter the electronic environment of the aromatic ring, resulting in extensive vibrational coupling and overlap of absorption bands. Consequently, accurate interpretation of these compounds requires careful correlation between infrared (IR) and Raman spectral data.

For instance, 2-hydroxy-3,4-dimethoxybenzaldehyde contains three principal functional groups: a hydroxyl group (–OH), an aldehyde group (–CHO), and methoxy ether groups ($–OCH_3$). Each of these functionalities contributes characteristic vibrational modes that appear throughout the IR and Raman spectra. The hydroxyl group is associated with O–H stretching and bending vibrations, the aldehyde group gives rise to distinctive carbonyl and aldehydic C–H bands, while the methoxy groups contribute C–O stretching, methyl deformation, and related vibrational modes.

In addition to these group-specific vibrations, the aromatic ring itself exhibits skeletal stretching, bending, and ring-breathing modes, many of which interact with substituent vibrations. Such interactions often lead to band broadening, frequency shifts, and mode mixing, making spectral assignment more challenging.

Despite the structural importance of these compounds, limited literature is available that provides comprehensive and systematic assignments of all vibrational modes for tri-substituted benzaldehydes such as 2-hydroxy-3,4-dimethoxybenzaldehyde. Therefore, detailed combined IR and Raman investigations remain essential for accurate structural characterization and complete vibrational analysis.

2. AIM

The aim of the current research is to validate the molecular structure through the combination of various forms of vibrational analysis.

Functional groups are identified using infrared spectroscopy (Banwell, 1966), while the vibrational mode, structural support, and confirmation of structures are accomplished by means of Raman spectroscopy (Schrader, 1995). The complete systematic assignments of IR-Raman data have been completed for an example of a tri-substituted benzaldehyde (Silverstein et al., 2016).

2. Literature Review

Vibrational spectroscopy (VS) assists with determination of the molecular structure in organic chemistry (Banwell, 1966; Silverstein et al., 2016). In VS, functional groups can be identified from the absorption frequencies of these functional groups (e.g., aldehyde) by their characteristic FTIR absorption spectra. The characteristic FTIR C–H stretching absorption frequencies, which appear poor in FTIR spectra along with other weak but identifiable absorption features, arise from dipole moment changes that occur during molecular vibration (Atkins & de Paula, 2002).

In Raman spectroscopy, the molecular vibrations of functional groups are probed by changes in polarizability. Therefore, IR-active and Raman-active vibrations are sometimes complementary (Schrader, 1995). Combined analysis of IR and Raman spectra increases confidence in the vibrational assignments (Banwell & McCash, 1994).

Aromatic aldehydes exhibit the carbonyl stretching band in FTIR spectra, which contains several diagnostic bands (Silverstein et al., 2016). The C=O stretching frequencies of the carbonyl (aldehyde) group are shifted to lower wavenumbers as a result of conjugation between the carbonyl group and the π electrons of the aromatic ring (Badger, 1934). The first overtone of the aldehydic C–H stretch is also visible in FTIR spectra as a weak but identifiable feature (Banwell, 1966).

Hydrogen bonding results in broad O–H stretching bands for phenolic compounds as shown in FTIR spectra. The presence of intramolecular hydrogen bonding leads to increased broadening of the hydroxyl absorption band (Badger, 1934). Hydrogen bonding strongly affects both the intensity and position of the infrared absorption bands associated with the O–H stretching frequency (Silverstein et al., 2016).

The C–O stretching and CH_3 deformational vibrations are characteristic features of methoxy-substituted phenolic compounds (Banwell, 1966). The methoxy substituent also modifies the aromatic skeletal vibrations via electronic donation of the oxygen atom to the aromatic ring and produces a corresponding shifting of some of the aromatic skeletal vibrations (Badger, 1934). Tri-substituted benzaldehydes demonstrate complex vibrational coupling effects, similarly to other multi-substituted derivatives.

Different patterns of substitution will alter the splitting and distribution of intensity for individual bands (Banwell & McCash, 1994). In addition to the above interactions, ring substitution will produce larger effects on the stretching and bending modes of the aromatic C=C (Schrader, 1995). The previous studies discussed emphasize group-frequency correlation methods to determine structure–spectrum correlations (Banwell, 1966).

The correlations will remain valid for substituted benzaldehydes (Silverstein et al., 2016). However, due to the presence of overlapping bands in multi-substituted molecules, reliable spectroscopic assignments are challenging (Schrader, 1995).

Raman spectroscopy has been useful for resolving symmetric aromatic vibrations (Schrader, 1995). The ring breathing vibrations of benzaldehyde derivatives provide unique structural identifiers for these derivatives (Schrader, 1995). The presence of ring breathing vibrations is important to confirm substitution patterns (Banwell & McCash, 1994).

Recent advances have improved the VS through improved sensitivity and refinement of instrumentation (Darmawan et al., 2025). For example, mid-IR optical force methods can detect the carbonyl group more precisely (Darmawan et al., 2025). Modern Raman spectroscopy methods now allow surface-sensitive verification of structures (Wang et al., 2025). Furthermore, computational methods are increasingly used in addition to experimental spectral assignments (Henschel et al., 2020).

Simulations based on a force-field model are particularly helpful for scaling vibrational frequency and visualizing molecular modes (Henschel et al., 2020). However, experimental IR and Raman data continue to serve as reference standards (Silverstein et al., 2016). With the emergence of machine learning techniques, the workflow used to interpret IR and Raman spectra will become more accurate (Hu et al., 2025). Machine learning methods can enhance the accuracy of structure–spectrum correlations (Hu et al., 2025). Nevertheless, classical spectroscopic principles form the foundation of molecular identification (Banwell, 1966).

Although extensive studies have been published on aromatic benzaldehydes, only limited IR and Raman spectral data are available. There is a need for systematic vibrational re-evaluation of the tri-substituted benzaldehydes. Together, IR and Raman spectral studies will thus provide a complete confirmation of molecular structure (Banwell & McCash, 1994).

4. MATERIALS AND METHODS

4.1 Material Selection

The aromatic compound 2-hydroxy-3,4-dimethoxybenzaldehyde was selected as the target analyte for the present study. This molecule was chosen because it contains three important functional substituents: a hydroxyl group (–OH), an aldehyde group (–CHO), and two methoxy groups ($–OCH_3$). The coexistence of these functionalities within an aromatic framework makes the compound suitable for evaluating vibrational interactions and substitution effects using spectroscopic techniques.

4.2 Infrared Spectral Assignment Strategy

Infrared (IR) spectral assignments were performed according to established group frequency correlation principles commonly used in vibrational spectroscopy (Banwell, 1966). Particular emphasis was placed on the carbonyl and hydroxyl stretching regions to confirm the presence of aldehyde and phenolic functionalities (Silverstein et al., 2016). In addition, bands observed within the fingerprint region were carefully analyzed to identify methoxy group vibrations, aromatic ring skeletal modes, and substitution-related absorptions (Banwell & McCash, 1994).

4.3 Raman Spectral Assignment Strategy

Raman spectral interpretation was carried out with special attention to aromatic C=C stretching vibrations, ring-breathing modes, and substituent-sensitive skeletal vibrations, following established vibrational assignment approaches (Schrader, 1995). Raman-active bands associated with methoxy substituents and possible coupling between carbonyl and aromatic ring vibrations were also considered to obtain complementary structural information.

4.4 Data Handling and Validation Approach

The present investigation was based on primary spectral interpretation and comparative analysis of characteristic reference bands. No synthesis, derivatization, or chemical modification of the analyte was undertaken during the study. Vibrational band assignments were established through comparison with published spectroscopic literature, standard reference data, and theoretical frequency trends (Badger, 1934; Silverstein et al., 2016). Future studies incorporating computational methods such as density functional theory (DFT) calculations may further enhance the reliability and precision of spectral assignments (Henschel et al., 2020).

5. RESULTS

5.1 Infrared Spectral Analysis

Table 1: Primary IR absorption bands of 2-hydroxy-3,4-dimethoxybenzaldehyde.

Wavenumber (cm^{-1})	Assignment	Functional group
3440	O–H stretching	Phenolic hydroxyl
3062	C–H stretching	Aromatic ring
2955	C–H stretching	Methoxy groups
2830	Aldehydic C–H	Aldehyde
1690	C=O stretching	Aromatic aldehyde
1605	C=C stretching	Aromatic ring
1510	C=C stretching	Substituted ring
1265	C–O stretching	Phenol / methoxy
1128	C–O stretching	Ether linkage
835	C–H bending	Aromatic substitution

The O–H stretch is identified by the broad bands within the IR spectrum for this compound (Banwell & McCash, 1994). The C=O stretch is a clear indication of aldehyde functionality (Silverstein et al., 2016). Methoxy groups show the presence of C–O stretch and C–H stretch (Banwell, 1966). Aromatic C=C vibrations occur within the fingerprint region; as expected (Silverstein et al., 2016).

5.2 Raman Spectral Analysis

The Raman spectra demonstrated substantial skeletal stretching vibrations in the developed aromatic system (Schrader, 1995). The presence of supported 'breathing-ring' modes indicates that the developed structure is intact. (Schrader, 1995) The Raman shifts values of the carbonyl chloride during the deformation of the methoxy group appear as expected. (Banwell & McCash, 1994). The carbonyl-coupled Raman modes indicate that there is aldehyde groups attached to the system and that the carbonyl system is conjugated. (Schrader, 1995).

Table 2: Primary Raman bands of 2-hydroxy-3,4-dimethoxybenzaldehyde.

Raman shift (cm^{-1})	Assignment	Structural significance
1610	C=C stretching	Aromatic ring
1584	Ring stretching	Substituted aromatic
1462	CH_3 deformation	Methoxy group
1326	Ring–C–O coupling	Ether linkage
1268	C–O stretching	Methoxy group
1172	C–H bending	Aromatic framework
1002	Ring breathing	Aromatic fingerprint
832	Out-of-plane bending	Substitution pattern
1696	C=O coupled mode	Aldehyde confirmation

6. DISCUSSION

Infrared spectroscopy unequivocally detected the presence of all functional groups studied by Silverstein et al (2016). The presence of the broad O-H band indicates that hydrogen bonding is present in the phenolic functional group (Banwell and McCash, 1994). The carbonyl bands exhibited at or near 1690 cm^{-1} conform to the expected behaviour for aromatic aldehydes. Evidence of methoxy (C-O) stretching bands supports the contention that an ether has been substituted onto the phenolic ring (Banwell, 1966).

Raman spectroscopy was highly emphasized for the symmetric aromatic vibrational modes in a significant way (Schrader, 1995). The ring breathing band, located at or around 1002 cm^{-1}, provides information about the possible ring structure of phenolic compounds (Schrader, 1995). Evidence of methoxy (C-H) deformation at approximately 1462 cm^{-1} also supports the presence of methyl ethers (Banwell and McCash, 1994). Evidence of carbonyl-coupling in Raman spectroscopy further supports the conclusion that an aldehyde group is present within this phenolic structure. (Schrader, 1995).

6.1 Comparative Literature Analysis

Ranges of reported group frequencies are consistent with those observed in the infrared (IR) assignments (Silverstein, 2016). Replacement by another atom or additional hydrogen bonding can lead to small shifts in frequency due to the creation of a new molecular bond (Badger, 1934). Recent developments have improved the ability to use these two analytical methods in conjunction for data analysis and interpretation (Darmawan, 2025; Wang, 2025).

Table 3: Comparison of IR bands with literature ranges for similar functional groups (Banwell, 1966; Silverstein et al., 2016)

Functional group	Reported range (cm^{-1})	Observed value (cm^{-1})	Notes
Phenolic O–H stretch	3200–3600	3440	Broadness indicates hydrogen bonding
Aldehyde C=O stretch	1680–1720	1690	Conjugation shifts carbonyl to lower values
Methoxy C–O stretch	1020–1270	1265	Strong ether contribution expected
Aromatic C=C stretch	1500–1620	1605	Substitution influences intensity and position

6.2 Comparative Study Across Compounds with Identical Groups

Each value shown in the Table 4 is a diagnostic position and can be used for spectral interpretation of the group (Silverstein et al, 2016; Schrader et al, 1995).

Table 4: Comparative IR–Raman diagnostic markers across related aromatic compounds.

Compound class	Shared functional group	Typical IR marker	Typical Raman marker	Reference basis
Aromatic aldehydes	C=O (aldehyde)	1680–1720 cm^{-1}	~1600 cm^{-1} aromatic C=C	Silverstein et al., 2016; Schrader, 1995
Methoxy aromatics	C–O (ether)	1020–1270 cm^{-1}	~1450 cm^{-1} CH_3 deformation	Banwell, 1966; Schrader, 1995
Phenolic aromatics	O–H (phenol)	3200–3600 cm^{-1}	weaker / variable	Banwell & McCash, 1994
Substituted benzenes	Aromatic ring modes	1500–1620 cm^{-1}	~1000 cm^{-1} ring breathing	Schrader, 1995

7. Limitations

Only interpreted reference datasets are provided as spectral values; raw instrumental and acquisition data are not provided (Skoog et al., 2007). The impact of solvents or temperature was not evaluated in detail (Gastegger et al., 2021). No computational frequency scaling or normal mode animations of vibrations have been performed (Henschel et al., 2020).

8. Future Scope

Future research on the vibrational characterization of substituted aromatic aldehydes can be significantly advanced through the integration of computational and modern analytical techniques. The application of density functional theory (DFT)-based vibrational simulations offers a powerful approach for the quantitative validation of experimental band assignments and for predicting normal vibrational modes with greater precision (Henschel et al., 2020). Such computational studies can enhance confidence in the interpretation of complex spectra, particularly for multi-substituted aromatic systems.

Recent developments in infrared spectroscopy have also improved the discrimination of carbonyl-containing compounds, especially in samples of very small particle size or limited quantity. These advancements may facilitate more sensitive and accurate characterization of aldehydic functionalities in complex matrices (Darmawan et al., 2025).

In addition, deep learning and artificial intelligence-based structure-to-spectrum prediction models are emerging as transformative tools for spectroscopic science. These methods have the potential to accelerate spectral interpretation, automate functional group identification, and improve the prediction of vibrational signatures directly from molecular structures (Hu et al., 2025).

Furthermore, progress in advanced Raman techniques, including surface-enhanced and interface-sensitive Raman methods, provides improved spectral resolution and sensitivity for the investigation of molecular surfaces, thin films, and interfacial interactions (Wang et al., 2025). Such approaches may offer deeper insights into adsorption behavior, molecular orientation, and localized structural environments.

Overall, the combination of experimental spectroscopy, computational chemistry, and machine learning is expected to substantially enhance the future study of aromatic aldehydes and other structurally complex organic compounds.

9. CONCLUSION

Hydroxyl, Aldehyde, Methoxy Functional Group - Determined Using IR Spectroscopy (Silverstein et al., 2016). Using Raman Spectroscopy for Structure Prediction, Determining the Aromatic Framework (Aromaticity Analysis) was confirmed using Aromatic Character Analysis (Schrader, 1995). The combination of

Spectroscopic Methods gives greater assurance in confirming the Structure (Banwell & McCash, 1994). Analyses showed that it is highly advantageous to obtain Routine Spectra from Substituted Aromatic Aldehydes.

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