

4-METHOXY SALICYLALDEHYDE: SPECTROSCOPIC AND COMPUTATIONAL INVESTIGATIONS

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ABSTRACT: 4-Methoxysalicylaldehyde was identified from the natural extract. The spectroscopic and electronic structural properties were investigated by FTIR, FT-Raman and UV-Vis spectroscopic techniques with help of quantum chemical calculations. The vibrational spectra were recorded in the mid IR region. The electronic spectrum was recorded in the region UV-Vis region. The observed values in vibrational and UV-Vis spectra were analyzed and assigned to various fundamental modes of vibration and transitions in the molecule respectively. The molecular geometry, vibrational spectra and electronic spectra were simulated using Density Functional Theory (DFT) based on B3LYP/6-311++G(d,p) basis set. The experimental and theoretical findings were shows excellent agreement, thereby to confirm the structure of 4-Methoxysalicylaldehyde.

Keywords: GC-MS, FT-IR, FT-Raman, UV-Vis, DFT calculations

1. Introduction

Benzaldehyde and its derivatives have received much attention due of their outstanding chemical, biological, pharmaceutical and physicochemical properties. 4-Methoxysalicylaldehyde is also known as 2-hydroxy-4-methoxy benzaldehyde with molecular formula $C_8H_8O_3$, which is one of the isomers of vanillin. From the structural point of view, it has one methoxy group in the para position and one hydroxyl group in the ortho position respective to the aldehyde group. Experimental and theoretical investigations on the benzaldehyde and its derivatives such as 4-Methoxybenzaldehyde, 3-chloro-4-methoxybenzaldehyde, 3-methoxy-4-hydroxybenzaldehyde, 2-hydroxy-3-methoxybenzaldehyde, 2-hydroxy-3-methoxy benzaldehyde thiosemicarbazone, 2-hydroxy-3-methoxy-N-(2-chloro-benzyl)-benzaldehyde-imines and 4-methoxybenzaldehyde-N-methyl-4-stilbazoliumtosylate were carried out by many researchers [1-14]. Though, 4-Methoxysalicylaldehyde has not been subjected to any experimental and theoretical investigations. For this reason, the present effort deals with spectroscopic and structural properties of 4-Methoxysalicylaldehyde. Moreover, an attempt has been made to identify 4-Methoxysalicylaldehyde from the methanolic extract of *Decalepis hamiltonii* yams using Gas Chromatography – Mass Spectrometry (GC-MS) techniques.

2. Materials and methods

2.1. Collection, selection and preparation of samples

Decalepis hamiltonii yams were freshly collected from Kalvarayan hills in Villupuram District, Tamil Nadu. It was taxonomically identified and authenticated by a botanist. The plant materials were cleaned and dried in shade at 30 – 40 °C temperature for 7-8 days. After drying process, it was crushed into fine powder with the aid of mechanical grinder and passed through a mesh sieve to ensure fine powdered particles. About 50 g of fine powdered sample was poured into 1000 mL of methanol within a soxhlet extraction apparatus. Then, it was allowed for continuous extraction process until the extractive material become colorless. The resulting crude methanolic extracts were filtered and stored in a refrigerator at 4 °C for further use of subsequent experiments.

2.2. Sample and experimental details

2 µl of methanolic extract of *Decalepis hamiltonii* yams were employed for Gas Chromatography – Mass Spectrometry (GC-MS) analysis. It was performed on a Perkin Elmer GC claurus 680 system and Gas Chromatograph interfaced to a Mass Spectrometer claurus 600 (EI) equipped with Elite-5MS fused silica capillary column (30.0m,0.25mmID,250µm df composed of 100% Dimethyl polysiloxane). For GC-MS detection, an electron ionization energy system with ionization energy of 70eV was used. Helium gas (99.999%) was used as the carrier gas at a constant flow rate of 1 ml /min and an injection volume 1 µl was employed (split ratio of 10:1). Injector temperature and Ion-source temperature was 240°C and 250°C respectively. The oven temperature was programmed from 60 °C, with an increase of 10°C/min to 300°C, ending with 6 min isothermal at 250°C. Mass spectra were taken at 70eV with a scan interval of 0.5 seconds and a fragment from 50 to 600 Da, total GC running time was 36 min. The relative percentage amount of each component was calculated by comparing its average peak area to the total areas. Turbo mass Ver5.4.2 software was adopted to handle mass spectra and chromatograms. The identification of components was carried out by referring to NIST-2008 mass spectral database.

Spectroscopically pure sample of 4-Methoxysalicylaldehyde in powder form was acquired from Spectrochem Pvt Ltd, India, with stated purity of 98% and it was used as such to record the spectral measurements. The FTIR spectrum was recorded in the mid IR region on a Perkin Elmer- spectrum Two FT-IR/ATR spectrometer system with 0.50 cm^{-1} resolution. The FT-Raman

spectrum was recorded in the mid IR region on a Bruker RFS-27 FT-Raman spectrometer with 2 cm^{-1} resolution using 1064 nm spectral line of Nd: YAG laser for excitation, operating at 100 mW power as excitation wave length. The electronic absorption spectrum was recorded on a Perkin Elmer-Lambda 35 UV Winlab V6.0 Spectrometer with a Bandwidth 0.5 - 4 nm (variable) in the UV-Visible region.

2.3. Computational details

All of the quantum chemical calculations were performed without any geometric limitation for 4-Methoxysalicylaldehyde at B3LYP level of theory included in Gaussian 09W program suite [15] together with 6-311++G(d,p) basis set. The molecular geometry optimizations, vibrational frequencies and electronic energies were calculated. All the computed structural values are true minimum on the potential energy surfaces proved by no imaginary values were found after the optimization. The vibrational assignments and electronic transitions were predicted by combining the outcome of Chemcraft program [16], which gives high degree of accuracy.

3. Results and discussion

3.1. Identification of compounds

GC-MS chromatogram of the natural extract of *Decalepis hamiltonii* yams shows the presence of 10 phytochemical compounds (Fig. 1). The unknown compounds were compared with known compounds stored in the reference database of National Institute Standard and Technology (NIST) library, which having 62000 patterns [17, 18]. With the aid of NIST library, 10 phytochemical compounds in the natural extract of *Decalepis hamiltonii* yams were characterized and identified as given in Table 1. It is the first report in this plant which revealed the presence of 10 bioactive compounds and hence to prove the therapeutic values of *Decalepis hamiltonii* yams.

Table 1. Phytochemical compounds identified from methanolic extract of *Decalepis hamiltonii* yams.

S.No.	RT (min)	Compound name	Molecular formula	Molecular weight (Da)	Peak area (%)
1	5.16	Ethylamine,1-Methyl-2(5-Methyl-1H-Pyrazol-3-yl)-	$\text{C}_7\text{H}_{13}\text{N}_3$	139	1.723
2	10.55	2-Furancarboxaldehyde,5-(Hydroxymethyl)-	$\text{C}_6\text{H}_6\text{O}_3$	126	15.711
3	11.12	4-Methoxysalicylaldehyde	$\text{C}_8\text{H}_8\text{O}_3$	152	6.650
4	11.49	4-Ethyl-2-Hydroxycyclopent-2-En-1-One	$\text{C}_7\text{H}_{10}\text{O}_2$	126	5.377
5	14.42	2-(1,2-Dihydroxyethyl)-9-(.Beta.-D-Ribofuranosyl) Hypoxanthine	$\text{C}_{12}\text{H}_{16}\text{O}_7\text{N}_4$	328	4.622
6	15.59	Adenosine, 1,2-Dihydro-2-Oxo-	$\text{C}_{10}\text{H}_{13}\text{O}_5\text{N}_5$	283	1.944
7	16.34	2-Undecene, 5-Methyl-	$\text{C}_{12}\text{H}_{24}$	168	20.362
8	18.15	. Beta.-D-Mannofuranoside, Methyl	$\text{C}_7\text{H}_{14}\text{O}_6$	194	27.426
9	19.66	Octadecanoic Acid	$\text{C}_{18}\text{H}_{36}\text{O}_2$	284	7.575
10	20.82	D-Glycero-L-Gluco-Heptose	$\text{C}_7\text{H}_{14}\text{O}_7$	210	8.611

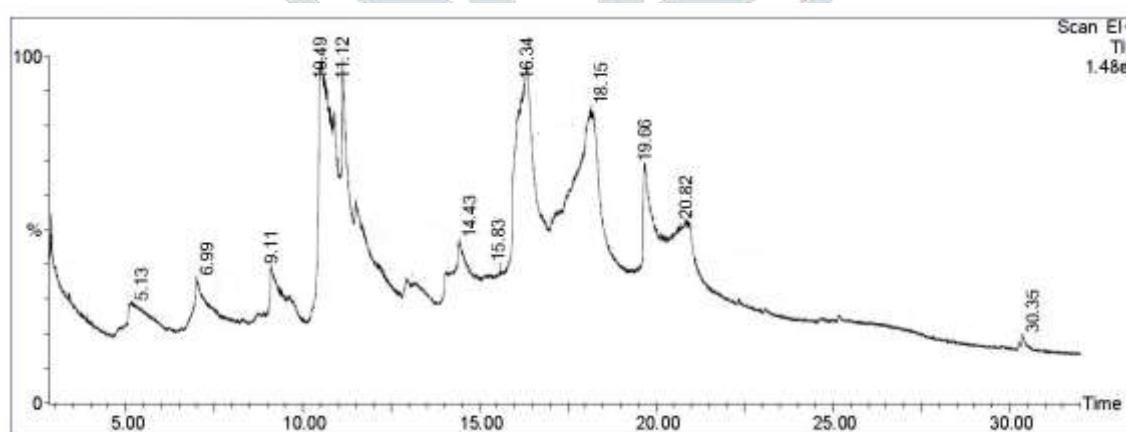


Fig. 1. GC-MS chromatogram of methanolic extracts of *Decalepis hamiltonii* yams

3.2. Optimized geometrical parameters

The prominent molecular geometry of 4-Methoxysalicylaldehyde was obtained at DFT/B3LYP level of theory with 6-311++G(d,p) basis set. The optimized molecular structure of 4-Methoxysalicylaldehyde along with atomic numbering is shown in Fig. 2, whereas the corresponding geometrical values are presented in Table 2. As the crystal structure of 4-Methoxysalicylaldehyde is not available in literature as yet, attempts have been made to compare with structurally similar compound [5, 6]. In the optimized molecular structure of 4-Methoxysalicylaldehyde, four types of bond lengths such as O-H, C-

O, C-C and C-H, and eight types of bond angles such as C-O-C, C-O-H, C-C-O, O-C-H, O-H-O, C-C-C, C-C-H and H-C-H were identified and calculated. The optimized C-O bond lengths were calculated in the range 1.426 – 1.231 Å and experimentally observed in the range 1.430 – 1.229 Å, whereas the optimized C-C-O bond angles are calculated in the range 124.48 – 115.35° and experimentally observed at 123.3°, which has been showed good correlation. The optimized O-H bond length and O-H-O bond angle calculated at 0.985 Å and 146.49° respectively. The O-C-H and H-C-H bond angles are calculated in the range 119.53 – 105.57° and 109.83 – 109.42° respectively. The C-O-C bond angle calculated at 119.36°, which shows better agreement with observed value at 117.6°. The O₃-H₈ is virtually bonded due to intra- and inter-molecular interaction, which has been calculated at 1.763 Å. The C-O-H bond angles calculated in the range 107.72 – 99.27° and observed at 95°. The C-C bond lengths were calculated in the range of 1.447 – 1.382 Å and experimentally observed in the range 1.427 – 1.382 Å, whereas, the optimized C-C-C bond angles are calculated in the range of 121.90 – 118.57° and experimentally observed in the range 121.5 – 118.9°, these value shows good in agreement. The C-H bond lengths were calculated in the range of 1.106 – 1.080 Å and experimentally observed in the range 1.100 – 0.910 Å, whereas, the optimized C-C-H bond angles are calculated in the range of 121.31 – 115.98° and experimentally observed in the range 120 – 106°. These values are found to be closely related to the standard values.

Table 2. Optimized molecular geometry of 4-Methoxysalicylaldehyde

Bond lengths (Å)	B3LYP	Bond lengths (Å)	B3LYP
O ₁ -C ₁	1.354	C ₃ -C ₄	1.390
O ₁ -C ₈	1.426	C ₄ -H ₁	1.082
O ₂ -C ₃	1.341	C ₅ -C ₆	1.382
O ₂ -H ₈	0.985	C ₅ -H ₂	1.080
O ₃ -C ₇	1.231	C ₆ -H ₃	1.086
C ₁ -C ₄	1.396	C ₇ -H ₄	1.106
C ₁ -C ₅	1.410	C ₈ -H ₅	1.088
C ₂ -C ₃	1.425	C ₈ -H ₆	1.094
C ₂ -C ₆	1.404	C ₈ -H ₇	1.094
C ₂ -C ₇	1.447	O ₃ -H ₈	1.763
Bond angles (°)	B3LYP	Bond angles (°)	B3LYP
C ₁ -O ₁ -C ₈	119.36	C ₁ -C ₅ -C ₆	118.57
O ₁ -C ₁ -C ₄	115.35	C ₁ -C ₅ -H ₂	121.31
O ₁ -C ₁ -C ₅	123.71	C ₃ -C ₂ -C ₆	118.65
O ₁ -C ₈ -H ₅	105.57	C ₃ -C ₂ -C ₇	120.71
O ₁ -C ₈ -H ₆	111.25	C ₂ -C ₃ -C ₄	119.84
O ₁ -C ₈ -H ₇	111.25	C ₆ -C ₂ -C ₇	120.65
C ₃ -O ₂ -H ₈	107.72	C ₂ -C ₆ -C ₅	121.90
O ₂ -C ₃ -C ₂	121.33	C ₂ -C ₆ -H ₃	118.56
O ₂ -C ₃ -C ₄	118.83	C ₂ -C ₇ -H ₄	115.98
O ₂ -H ₈ -O ₃	146.49	C ₃ -C ₄ -H ₁	120.05
O ₃ -C ₇ -C ₂	124.48	C ₆ -C ₅ -H ₂	120.13
O ₃ -C ₇ -H ₄	119.53	C ₅ -C ₆ -H ₃	119.54
C ₇ -O ₃ -H ₈	99.27	H ₅ -C ₈ -H ₆	109.42
C ₄ -C ₁ -C ₅	120.95	H ₅ -C ₈ -H ₇	109.42
C ₁ -C ₄ -C ₃	120.10	H ₆ -C ₈ -H ₇	109.83
C ₁ -C ₄ -H ₁	119.85	-	-

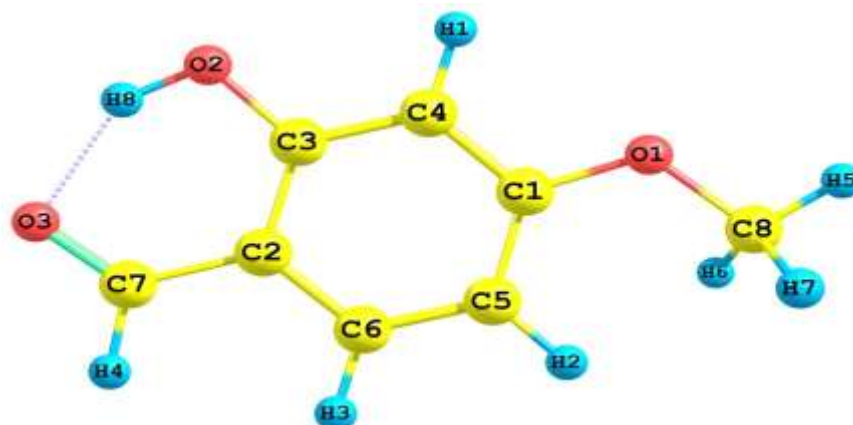


Fig. 2. Optimized molecular structure of 4-Methoxysalicylaldehyde

3.3. Vibrational spectral analysis

From the structural point of view, 4-Methoxysalicylaldehyde belongs to C_1 point group symmetry, which has 19 atoms and 51 fundamental vibrational modes based on $(3N-6)$ vibrational degrees of freedom. The detailed experimental and theoretical FT-IR and FT-Raman frequencies for different fundamental modes of vibrations were summarized in Table 3. The experimental and theoretical vibrational spectra were shown in Figs. 3 and 4. The vibrational spectra showed the distinctive bands of OH, CH_3 , CH, CO and CC vibrations, also the bending vibrations of aforementioned groups were observed in the finger print region. The vibrational assignments of the 4-Methoxysalicylaldehyde were aided by animation option of the Chemcraft program without any anomaly.

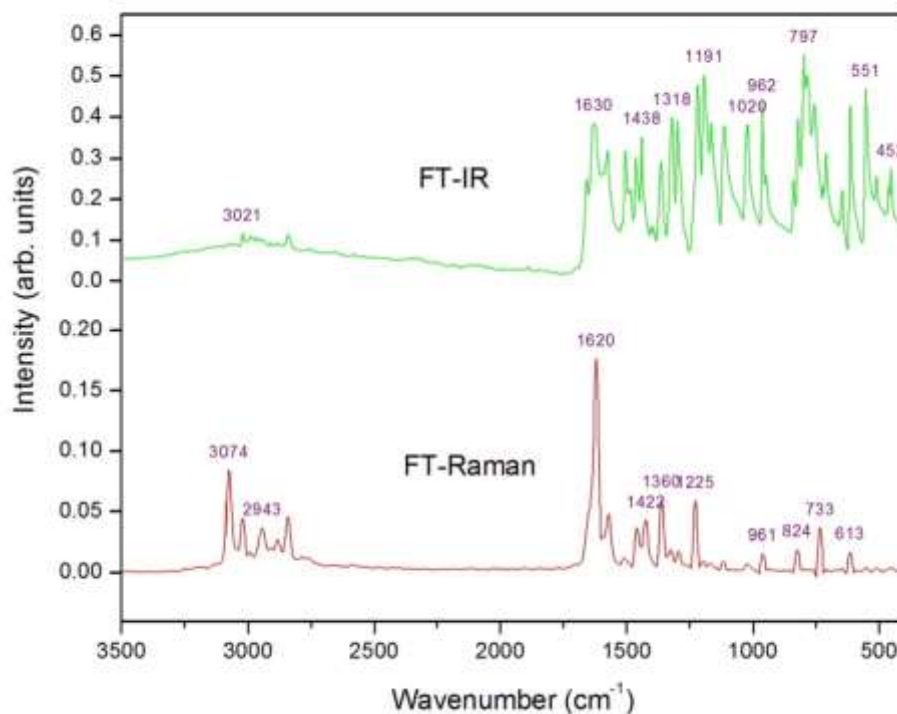


Fig. 3. Experimental vibrational spectra of 4-Methoxysalicylaldehyde

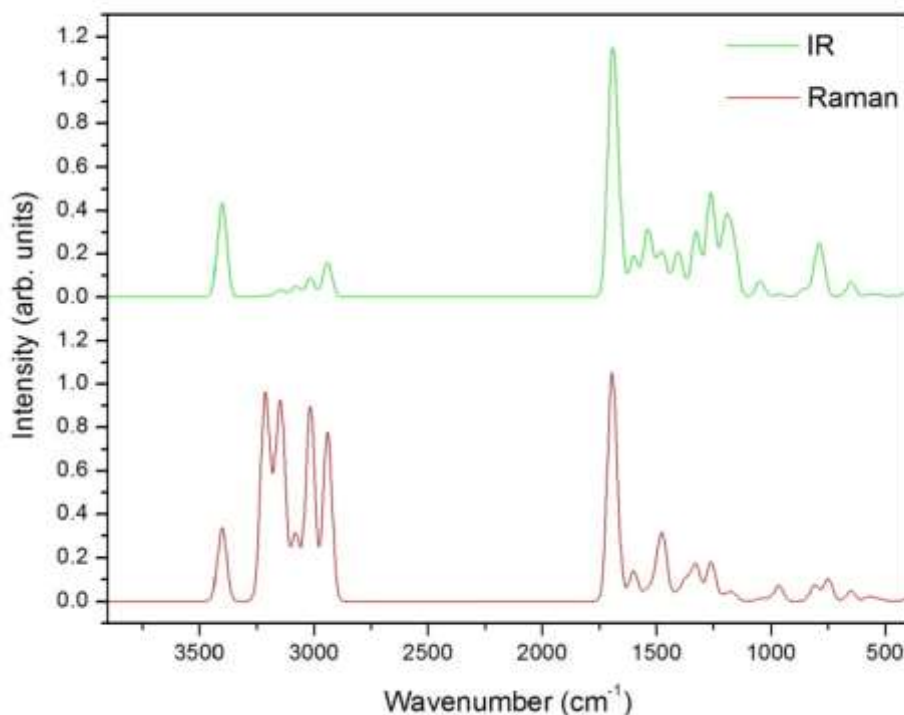


Fig. 4. Theoretical vibrational spectra of 4-Methoxysalicylaldehyde

Table 3. Experimental and theoretical vibrational wavenumbers of 4-Methoxysalicylaldehyde

Modes	Experimental wavenumbers (cm ⁻¹)		Theoretical wavenumbers (cm ⁻¹)	Vibrational assignments
	FT-IR	FT-Raman		
1			3402	ν OH
2			3220	ν CH
3			3207	ν CH
4			3162	ν CH
5			3142	ν CH + ν_{as} CH ₃
6	3073	3075	3080	ν CH + ν_{as} CH ₃
7	3021	3021	3016	ν_s CH ₃
8	2990	2944	2940	ν CH
	2840	2882		(1458+1422)
		2842		(1438+1401), (1619+1226)
9			1695	ν C=O
10	1665, 1630	1619	1668	ν C=O
11	1574	1570	1599	ν CC
12			1539	ν CC + δ_s CH ₃
13	1503	1508	1504	ν CC
14			1495	δ_{as} CH ₃
15			1477	δ_{as} CH ₃
16	1461	1458	1471	β CH + δ_{as} CH ₃
17	1438	1422	1422	β CH + δ_{as} CH ₃
18	1401		1401	β CH
19	1361	1359	1369	ν CC + β CH + δ_s CH ₃
20	1318	1323	1325	ν CO + β CH + δ_s CH ₃
21	1296	1292	1261	ν CC + β CH + δ_s CH ₃
22			1254	β CH + β OH + ν CO
23	1216	1226	1208	β CH + β OH + δ_s CH ₃
24	1191	1193	1190	β CH + β OH
25	1162		1166	β CH
26	1113	1115	1159	ν CO + β CH
27			1048	ν CO + β CH
28	1020	1020	1014	β CH
29	962	960	966	ν CO + γ CH
30			940	γ CH + δ Ring
31	839		860	γ CH
32	820	823	809	γ CH + δ Ring
33	797		793	γ OH
34	783		779	γ OH
35	756	734	749	γ CH + γ OH
36	709		697	γ CH + γ OH
37			656	γ CH + δ Ring
38	645, 613	614	648	δ C=O + δ Ring
39	551	550	569	γ OH
40	509		523	γ OH
41	452		464	δ Ring
42			408	δ C-OH
43		360	371	δ C-OH + δ_{as} O-CH ₃
44			327	δ CH + δ Ring
45		269	278	δ CH + δ C-OH + δ_{as} O-CH ₃ + δ C=O
46			256	δ CH + δ_{as} CH ₃

47		227	δ CH + δ_{as} CH ₃
48		209	δ CH + δ_{as} CH ₃ + δ C=O
49		204	δ CH + δ_{as} CH ₃
50	100	116	δ_{as} O-CH ₃
51	66	73	δ_{as} CH ₃ + δ C=O

ν_s - symmetric stretching; ν_{as} - symmetric stretching; δ - bending; β - in-plane bending; γ - out-of-plane bending.

3.3.1. O-H vibrations

The O-H group gives rise to three vibrations such as stretching, in-plane bending and out-of-plane bending vibrations. The OH group vibrations are likely to be most sensitive to the environment, so they show significant effect in the vibrational spectra of the aromatic system, which may decrease or increase the wavenumber for OH stretching and bending vibrations. The unassociated hydroxyl groups are expected to appear in the range 3700 – 3550 cm⁻¹. As aforementioned, the OH stretching vibration decreases from 3700-3550cm⁻¹ to 3550 – 3200 cm⁻¹ region for five and six membered ring system [19, 20]. The OH in-plane-bending vibrations [21, 22] usually appear in the expected region 1250 – 1150 cm⁻¹ and the OH out-of-plane vibrations appear in the expected region 710 – 517 cm⁻¹. In the present attempt, the OH stretching vibration can be effortlessly predicted and assigned at 3402 cm⁻¹ in the isolated state. Though, simplified experimental model does not consider the inter- and intra-molecular interaction in the solid state. Thus it is expected, the OH stretching vibrational band has not observed in experimental vibrational spectra. The OH in-plane bending vibrations were observed and assigned at 1216, 1191 cm⁻¹ in the FT-IR spectrum and at 1226, 1193 cm⁻¹ in the FT-Raman spectrum, the corresponding bands are calculated in the range 1254 – 1190 cm⁻¹. The OH out-of-plane bending vibrations were observed and assigned at 797, 783, 756, 709, 551, 509 cm⁻¹ in the FT-IR spectrum and at 734, 614, 550 cm⁻¹ in the FT-Raman spectrum, the corresponding bands are calculated in the range 793 – 523 cm⁻¹.

3.3.2. O-CH₃ vibrations

In general, the methyl groups are referred to as electron giving group in the aromatic compounds, which have been rousing to exist two asymmetric stretching and one symmetric stretching vibration. In the aromatic methoxy compounds, CH₃ asymmetric stretching vibrations may arises at 2985±20 cm⁻¹ and 2955±20 cm⁻¹, while the CH₃ symmetric stretching vibrations may arises at 2845±45 cm⁻¹ [23]. In the present study, the CH₃ asymmetric stretching vibrations observed at 3073 cm⁻¹ in the FT-IR spectrum and at 3075 cm⁻¹ in the FT-Raman spectrum, which is assigned to CH₃ asymmetric stretching vibrations. These bands are theoretically calculated at 3142 and 3080 cm⁻¹. The CH₃ symmetric stretching vibration observed at 3021 cm⁻¹ in the vibrational spectra and theoretically calculated at 3016 cm⁻¹, which is assigned to CH₃ symmetric stretching vibrations. The CH₃ asymmetric and symmetric bending vibrations expected to appear in the region 1465 - 1440 cm⁻¹ and 1390 - 1370 cm⁻¹ respectively [24]. In the 4-Methoxysalicylaldehyde, the CH₃ asymmetric bending vibrations were observed at 1461, 1438 cm⁻¹ in the FT-IR spectrum and at 1458, 1422 cm⁻¹ in the FT-Raman spectrum, which is assigned to CH₃ asymmetric bending vibrations. The CH₃ symmetric bending vibrations were observed at 1361, 1318, 1296, 1216 cm⁻¹ in the FT-IR spectrum and at 1359, 1323, 1292, 1226 cm⁻¹ in the FT-Raman spectrum, which is assigned to CH₃ symmetric bending vibrations. The CH₃ asymmetric and symmetric bending vibrations computationally calculated and assigned in the range 1495 – 1422 cm⁻¹ and 1369 – 1208 cm⁻¹ respectively.

3.3.3. C-H and C-C vibrations

In the vibrational spectra, aromatic compounds show evidence of several bands in the range 3100-3000 cm⁻¹ due to CH stretching vibrations. The CH bending vibrations are appear at two separate regions 1450 – 1000 cm⁻¹ and 1000 – 750 cm⁻¹ due to in-plane and out-of-plane bending vibrations respectively [25, 26]. In the present study, the CH stretching vibrations observed and assigned at 3073, 2990 cm⁻¹ in the FT-IR spectrum and at 3075, 2944 cm⁻¹ in the FT-Raman spectrum, which is calculated in the range 3220 – 2940 cm⁻¹. The in-plane bending vibrations observed and assigned in the range 1461 – 1020 cm⁻¹ in the FT-IR spectrum and 1458 – 1020 cm⁻¹ in the FT-Raman spectrum, which is calculated in the range 1471 – 1014 cm⁻¹. Meanwhile the CH out-of-plane bending vibrations observed and assigned in the range 962 – 709 cm⁻¹ in the FT-IR spectrum and 960 – 734 cm⁻¹ in the FT-Raman spectrum, which is calculated in the range 966 – 656 cm⁻¹.

The C-C stretching vibration of aromatic compounds usually appears in the range of 1650-1200 cm⁻¹ [27, 28]. In conjugated systems, the vibrational wavenumbers of C-C stretching is usually lesser than isolated C-C groups. In the vibrational spectra, two or three C-C stretching vibrational bands are observed for aromatic six membered rings due to skeletal vibrations. The C-C vibration varies depending upon the attachment of substitution group on the ring system. In the present study, C-C stretching vibrations observed and at 1574, 1503, 1361, 1296 cm⁻¹ in the FT-IR spectrum and at 1570, 1508, 1359, 1292 cm⁻¹ in the FT-Raman spectrum, which is calculated in the range 1599 – 1261 cm⁻¹.

3.3.4. C=O and C-O vibrations

The double bond in the carbonyl group (C=O) is formed by $p_\pi - p_\pi^*$ bonding, because of different electro negativities of carbon and oxygen atoms and lone pair bonding electrons are not evenly distributed among these atoms. The C=O stretching vibrations are usually appears at expected region 1850 – 1550 cm⁻¹ [29]. In the present study, these vibrations observed and assigned at 1665, 1630 cm⁻¹ in the FT-IR spectrum and at 1619 cm⁻¹ in the FT-Raman spectrum, which is calculated at 1695, 1668 cm⁻¹. The C=O bending vibrations observed and assigned at 645, 613 cm⁻¹ in the FT-IR spectrum and at 614 cm⁻¹ in the FT-Raman spectrum. In general, the C-O stretching vibrations in alcohols and phenols [30] appear in the expected region 1260 - 1000 cm⁻¹. The C-O stretching vibrations may be coupled with the adjacent C-C stretching vibrations. In the present study, C-O stretching vibrations observed and assigned at 1318, 1113, 962 cm⁻¹ in the FT-IR spectrum and at 1323, 1115, 960 cm⁻¹ in the FT-Raman spectrum, which is computationally calculated in the range 1325 - 966 cm⁻¹.

3.4. UV- Vis spectral analysis

The experimental UV-Vis spectrum of 4-Methoxysalicylaldehyde was measured in methanol and theoretically simulated at TD-DFT calculation method with B3LYP / 6-311++G (d,p) basis set. The calculated values such as absorption wavelengths (λ), excitation energies (E) and oscillator strength (f) were presented in Table 4, along with experimental values. The experimental and theoretical electronic spectra of the title compound were shown in Figs. 5 and 6. The experimental UV-Vis spectrum shows three bands at 314, 278 and 230 nm, whereas the theoretically calculated at 305, 302 and 268 nm. The experimental and theoretical values shows good agreement, thereby the maximum wavelength absorption (λ_{\max}) will take place at 278 nm in experimental method and 268 nm in theoretical method.

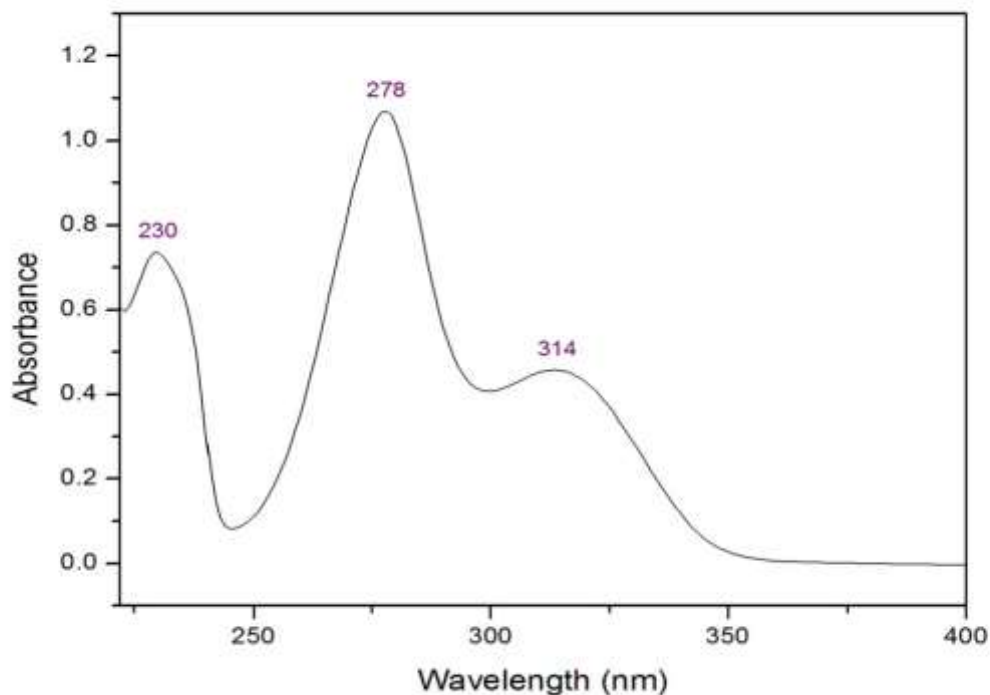


Fig. 5. Experimental electronic spectrum of 4-Methoxysalicylaldehyde

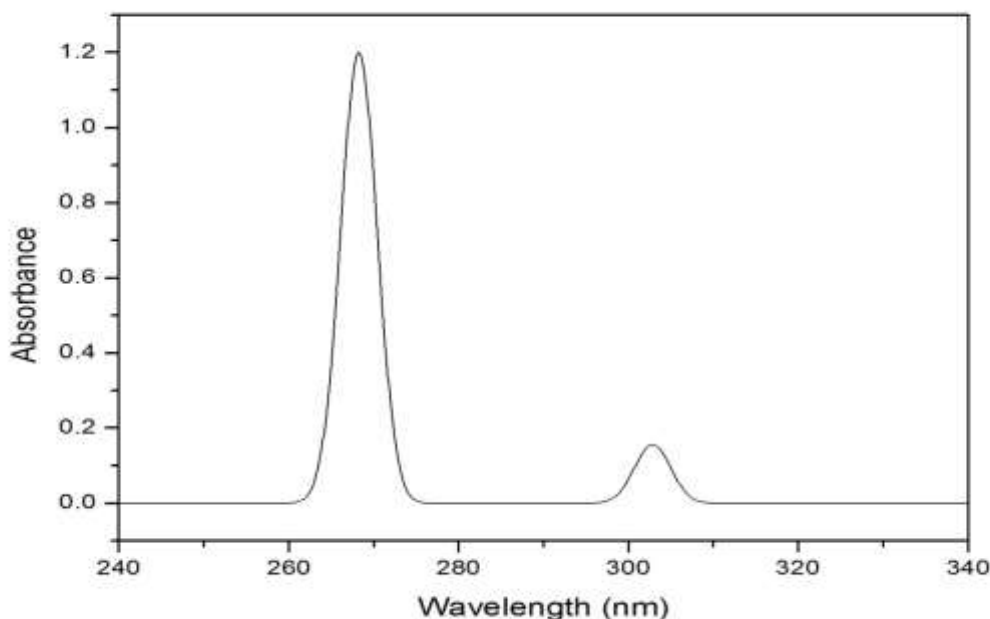


Fig. 6. Theoretical electronic spectrum of 4-Methoxysalicylaldehyde

Table 4. Experimental and calculated electronic parameters of 4-Methoxysalicylaldehyde

State	Experimental values		TD-DFT / 6-311++G (d,p)		
	λ (nm)	Abs.	λ (nm)	E (eV)	f
S ₁	314	0.457	305	4.060	0.0004
S ₂	278	1.069	302	4.093	0.0453
S ₃	230	0.736	268	4.622	0.3511

4. Conclusions

4-Methoxysalicylaldehyde was identified from the natural extract of *Decalepis hamiltonii* using GC-MS techniques. The optimized molecular geometry, vibrational assignments and electronic transitions for 4-Methoxysalicylaldehyde were investigated by spectroscopic studies such as FT-IR, FT-Raman and UV-Vis techniques with the help of high level of quantum chemical calculations. The vibrational spectra were confirmed the presence of OH, CH₃, CH, CC, C=O and CO groups in the 4-Methoxysalicylaldehyde. The UV-Vis spectrum gives an idea about electronic transitions in the molecule, which proves the molecular stability. The obtained experimental and theoretical findings exhibit an excellent correlation in confirmation of the molecular structure of 4-Methoxysalicylaldehyde.

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