

Vibrational analysis of flavone

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Abstract

In this study, the experimental and theoretical study on the structures and vibrations of flavone are presented. FT-IR and FT-Raman spectra of the molecule have been recorded in the 400–4000 cm^{-1} region and the 5–3500 cm^{-1} region, respectively. The molecular geometry and vibrational frequencies of flavone in the ground state have been calculated by using Density Functional method (B3LYP) in conjunction with 6-311++G(d,p) and 6-31++G(d) as basis sets.

Key Words: Infrared spectra, Raman Spectra, Hartree-Fock, Density functional theory, Flavone.

1. Introduction

Flavonoids are a large group of plant secondary metabolites that share a basic phenylbenzopyrone feature and are found in all vascular plants where they occur in several structurally and biosynthetically related classes [1, 2]. They are important constituents of the human diet [1, 3] and can also be found in expressive amounts in many medicinal plants [1, 4]. Flavonoid is any member of a class of widely distributed biological natural products containing aromatic heterocyclic skeleton of flavan but no nitrogen. Generally, flavonoids are biological pigments providing colors from red to blue in flowers, fruit and leaves. Besides their coloring in plants, flavonoids have important roles in the growth and development of plants; protection against UV-B radiation; forming antifungal barriers; antimicrobial, insecticidal and oestrogenic activities; and plant reproduction. Flavonoids also exhibit a wide range of biological properties including anti-microbial, insecticidal and oestrogenic activities [5].

Flavone has been investigated by Raman and surface-enhanced Raman spectra [6], Gas phase infrared spectra [7]. Mantas et al. [8] performed ab initio conformational analysis of flavone and related compounds. In this study, conformational analysis was investigated at HF/STO-3G level of theory and optimized geometric

parameters and vibrational spectra were calculated at HF level with STO-3G and 3-21G basis sets. However, in that study only values of the flavone frequencies were given. Waller et al. [9] crystallized and structurally characterized a single crystal of flavone. The vibrational frequencies for flavone and some deuterated analogues have been calculated from the conformational analysis of flavone using the semi-empirical AM1 method and compared with experimental values by Vrielynck et al. [10]. Vrielynck et al. [11] calculated conformational analysis of flavone by vibrational and quantum mechanical studies. These calculations used combined molecular mechanics (MMX), semi-empirical (AM1) and ab initio calculations. Although semi-empirical methods proved its usefulness in practice to facilitate the IR identifications, the performance of semi-empirical methods can not satisfy modern criteria of theoretical FT-IR spectral predictions. The IR spectra computed with Hartree-Fock (HF) and density functional theory (DFT) methods were in much better agreement with the observed IR spectrum: the correlation between the calculated and experimental vibration frequencies was characterized by the coefficients for all DFT methods higher than HF method. The calculated absolute band intensities were satisfactorily matched with the observed relative intensities as well.

In the present work, we report the results of calculated and experimental (IR and Raman) spectra of the flavone molecule using the DFT approximations. To the best of our knowledge, detailed quantum chemical calculations of the vibrational spectra of flavone have not been reported. Therefore, the present investigation was undertaken to study the vibrational spectra of this molecule completely and to identify the various modes with greater wavenumber accuracy. Density Functional Theory (DFT) calculations have been performed to support our wavenumber assignments. Furthermore, we interpreted the calculated spectra of in terms of total energy distributions (TEDs) and made the assignment of the experimental bands based on the results of the TED analysis.

2. Experimental

Flavone samples were purchased from Sigma-Aldrich Chemical Company with a stated purity of greater than 98% and it was used as such without further purification. The flavone sample is in powder form at room temperature. The infrared spectrum of the sample was recorded between 400–4000 cm^{-1} on a Mattson 1000 FTIR spectrometer which was calibrated using polystyrene bands. The sample was prepared as a KBr disc. The FT-Raman spectrum of the sample was recorded between 5–3500 cm^{-1} regions on a Bruker FRA 106/S FT-Raman instrument using 1064 nm excitation from a Nd:YAG laser. The detector is a liquid nitrogen cooled Ge detector.

3. Computational details

The molecular structure of flavone (in vacuum) in the ground state is optimized by HF and B3LYP with the 6-311++G(d,p) and 6-31++G(d) basis sets. Vibrational frequencies are calculated with DFT (B3LYP) approximation and then scaled by corresponding scaling factors. All the calculations are performed by using Gauss-view molecular visualization program and Gaussian 03W program package on a personal computer [12, 13]. These calculations are valuable to gain insight into the vibrational spectroscopy and molecular parameters of flavone structure.

4. Results and discussion

4.1. Conformational analysis

While the conjugation interaction between the C ring and A and B rings tends to prefer a planar structure, the steric repulsion between the ortho-ring hydrogens favors a nonplanar structure. The equilibrium geometry of the molecule results from a balance between these two effects. Figure 1 shows the variation of torsional barriers with the dihedral angles. The calculated relative energies and dipole moment for torsional angle are given in Table 1. The torsional barrier for phenyl rotation computed at the B3LYP and HF with 6-31++G(d,p) basis set corresponds to a low-transition state at 0° and high-transition state at 90° . For both models, the relative energy of corresponding molecule displays the same trends with the uniform shape of torsional dependence.

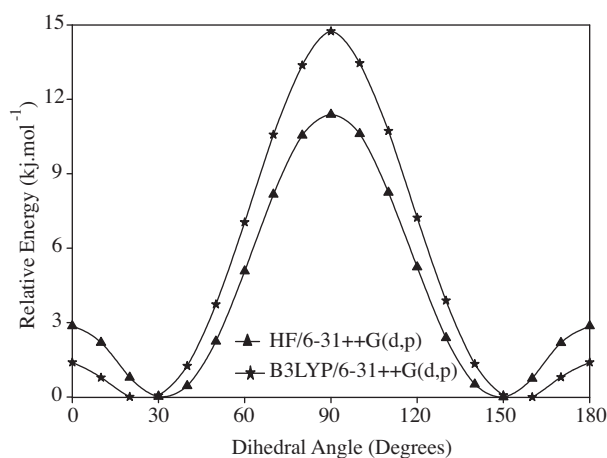


Figure 1. Torsional barriers of the flavone.

B3LYP/6-31++G(d,p) level of theory calculations predicted the dihedral angle (OCCC) as 20.37° , while the corresponding predictions were 20.67° (B3LYP/6-31++G(d,p)) and 28.18° (HF/6-31++G(d,p)) for flavone. The dihedral angle is determined at about 30° via the HF method, and at about 20° via the B3LYP method. This angle is experimentally determined as 10.53° in single crystal diffraction study for flavone [9]. Mantas et al. [8] calculated it as 20.82° for HF/STO-3G level of theory.

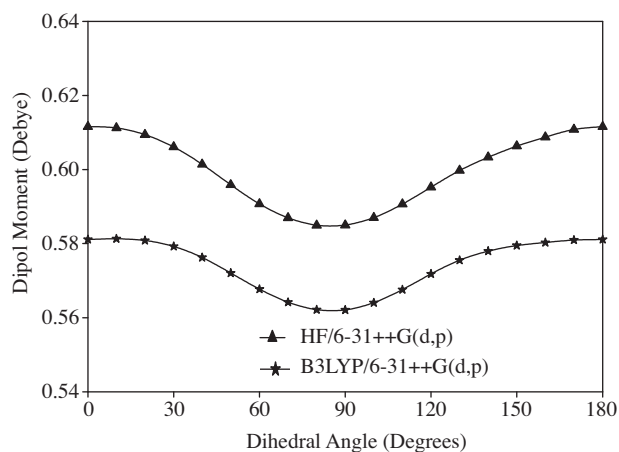
The calculated dipole moment results are shown in Table 1. The variation of dipole moment with the dihedral angle for flavone is shown in Figure 2. The dipole moments are calculated at B3LYP and HF with 6-31++G(d,p) basis set.

4.2. Geometry optimization

Optimized molecular structure of the flavone was calculated using RHF and B3LYP levels of theory using 6-31++G(d,p) and 6-311++G(d,p) standard basis sets. Optimized molecular structure of flavone is given in Figure 3. Calculated geometric parameters and definitions of the natural coordinates for the molecules are summarized in Table 2. X-ray data of flavone is reported by Waller et al. [9].

Table 1. Low and high energy barriers of phenyl rotation computed at various levels of theory for flavone.

		Minimum Energy Conformation	Transition State	
			Low (E_0)	High (E_{90})
Energy (Hartree)	HF	-723.624177905	723.611046659	723.607800553
	6-31++G(d,p)			
	B3LYP	-728.114106428	728.110468847	728.105385922
ΔE (kcal/mol)	HF	0.0	8.24	10.27
	6-31++G(d,p)			
	B3LYP	0.0	2.28	5.47
Dipol Moment (D)	HF	0.59	0.61	0.58
	6-31++G(d,p)			
	B3LYP	0.60	0.58	0.56
	6-31++G(d,p)			

**Figure 2.** Dihedral angle-Dipole moment curves of the flavone.

The C_4 - C_{14} bond distances are between 1.475–1.490 Å. This distance is variously determined as: 1.475 Å (B3LYP/6-31++G(d,p)), 1.474 Å (B3LYP/6-311++G(d,p)), 1.481 Å (HF/6-31++G(d,p)) and 1.481 Å (HF/6-311++G(d,p)) for both flavone. The dihedral angle between the phenyl and the pyrone ring is small (8.9 Å), as expected in the generally preferred conformation of flavones. The small dihedral angle results in a relatively short C_4 - C_{14} bond length of 1.472 (2) Å is consistent with bond lengths and dihedral angles as found in other

flavones [14]. Flavone-3/-sulfonamide has a dihedral angle of 8.2° and the C_4-C_{14} bond length of $1.478(3) \text{ \AA}$ [15]. In 5-hydroxyflavone, the dihedral angle is 5.2° and the C_4-C_{14} bond length is 1.465 \AA [16]. 5,7-Dihydroxy-4/-methoxyflavone with a dihedral angle of 3.1° has a C_4-C_{14} bond length of 1.453 \AA [17]. However, in 2/-methyl-3/-nitroflavone, the dihedral angle is 139.8° and the C_4-C_{14} bond length is 1.491 \AA [18], and in 5,4/-dihydroxy-3,6,7,8- tetramethoxyflavone a large dihedral angle of 164.4° and a C_4-C_{14} bond length of 1.503 \AA were reported [19].

Table 2. Bond lengths and bond angles for flavone.

Bond Lengths (\AA)	B3LYP	HF	X-RAY [6]	Bond Angles ($^\circ$)	B3LYP	HF	X-RAY [6]
	6-311++G(d,p)	6-311++G(d,p)			6-311++G(d,p)	6-311++G(d,p)	
C ₁ -C ₂	1.455	1.460	1.448	C ₂ -C ₁ -C ₆	113.9	113.8	114.1
C ₁ -C ₆	1.481	1.479	1.475	C ₂ -C ₁ -O ₂₆	123.2	123.2	123.5
C ₁ -O ₂₆	1.226	1.197	1.232	C ₆ -C ₁ -O ₂₆	122.7	122.9	122.3
C ₂ -C ₄	1.355	1.335	1.354	C ₁ -C ₂ -C ₄	122.5	121.6	122.4
C ₄ -C ₁₄	1.475	1.482	1.475	C ₂ -C ₄ -C ₁₄	125.8	125.3	125.8
C ₄ -O ₂₅	1.361	1.341	1.367	C ₂ -C ₄ -O ₂₅	121.8	122.5	122.2
C ₅ -C ₆	1.398	1.381	1.393	C ₁₄ -C ₄ -O ₂₅	112.2	112.1	111.9
C ₅ -C ₁₂	1.396	1.391	1.395	C ₆ -C ₅ -C ₁₂	121.5	121.3	121.6
C ₅ -O ₂₅	1.371	1.352	1.374	C ₆ -C ₅ -O ₂₅	121.8	121.9	122.3
C ₆ -C ₇	1.403	1.398	1.405	C ₁₂ -C ₅ -O ₂₅	116.5	116.6	115.9
C ₇ -C ₉	1.384	1.372	1.374	C ₁ -C ₆ -C ₅	119.6	119.3	119.6
C ₉ -C ₁₀	1.403	1.398	1.397	C ₁ -C ₆ -C ₇	121.8	121.7	121.8
C ₁₀ -C ₁₂	1.386	1.374	1.379	C ₅ -C ₆ -C ₇	118.5	118.8	118.5
C ₁₄ -C ₁₅	1.402	1.391	1.400	C ₆ -C ₇ -C ₉	120.5	120.4	120.2
C ₁₄ -C ₂₃	1.403	1.391	1.399	C ₇ -C ₉ -C ₁₀	120.2	120.4	120.1
C ₁₅ -C ₁₇	1.391	1.384	1.391	C ₉ -C ₁₀ -C ₁₂	120.6	120.8	120.9
C ₁₇ -C ₁₉	1.393	1.384	1.393	C ₅ -C ₁₂ -C ₁₀	118.8	118.7	118.4
C ₁₉ -C ₂₁	1.394	1.385	1.380	C ₄ -C ₁₄ -C ₁₅	120.4	120.1	121.1
C ₂₁ -C ₂₃	1.390	1.383	1.385	C ₄ -C ₁₄ -C ₂₃	120.7	120.7	119.3
				C ₁₅ -C ₁₄ -C ₂₃	118.7	119.1	119.4
				C ₁₄ -C ₁₅ -C ₁₇	120.4	120.3	120.0
				C ₁₅ -C ₁₇ -C ₁₉	120.3	120.2	120.1
				C ₁₇ -C ₁₉ -C ₂₁	119.6	119.7	119.5
				C ₁₉ -C ₂₁ -C ₂₃	120.2	120.1	121.2
				C ₁₄ -C ₂₃ -C ₂₁	120.5	120.3	119.6
				C ₄ -O ₂₅ -C ₅	120.1	120.7	119.1

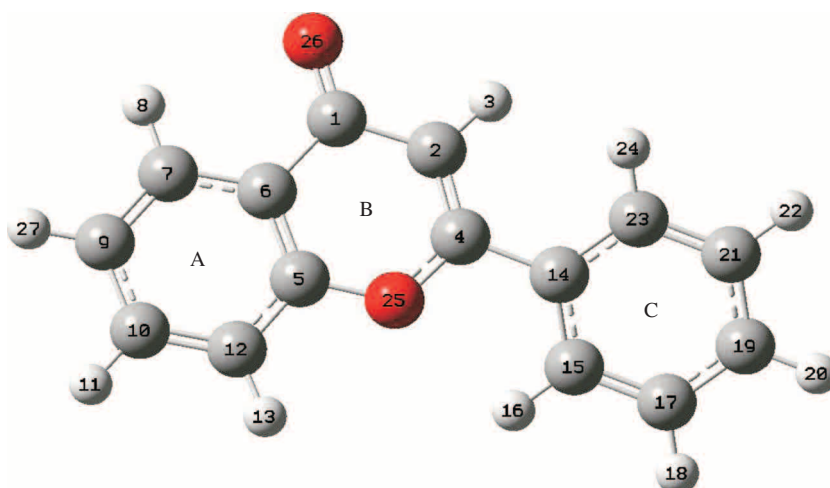


Figure 3. Flavone structure and atoms numbering.

The average C-C bond lengths for rings A and C are 1.394 Å and 1.383 Å for 6-methylflavone [14]. The average C-C bond lengths of the A, B and C rings are 1.395 Å, 1.422 Å and 1.396 Å in flavone for the B3LYP/6-311++G(d,p) calculation. Calculated C-H bond lengths are in the range of 1.070 Å–1.086 Å in flavone for B3LYP and HF respectively. C=O bond lengths are between 1.226 Å–1.234 Å and 1.197 Å–1.203 Å in the flavone for B3LYP and HF respectively. All aromatic ring angles are almost 120° for flavone.

4.3. Vibrational analysis

Flavone consists of 27 atoms, which has 75 normal modes. The 75 normal modes of the flavone have been assigned according to the detailed motion of the individual atoms. This molecule belongs to C_1 symmetry group. To the best of our knowledge, there are no detailed quantum chemical studies for the FT-IR and FT-Raman spectra of flavone. Scale factors were used to fit the calculated wavenumbers with those of the observed ones. The FT-IR (Figure 4) and FT-Raman (Figure 5) spectra of flavone are given. The experimental FT-IR

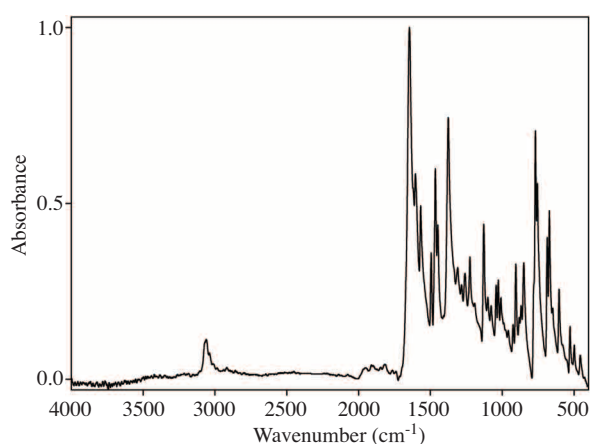


Figure 4. Infrared spectra of the Flavone.

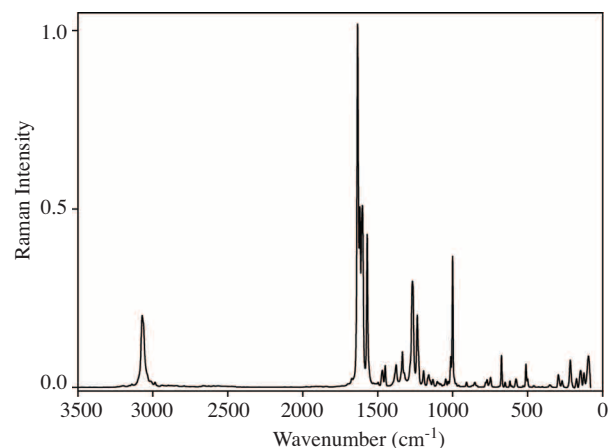


Figure 5. Raman spectra of the Flavone.

and FT-Raman wavenumbers are tabulated in Table 3 together with the calculated wavenumbers. As seen in Table 3 IR absorption intensities of flavone are consistent with the PED results [20].

The theoretical Raman intensities (I_i^R) can be derived from the computed Raman scattering activities using the equations

$$I_i^R = C (v_0 - v_i)^4 \cdot v_i^{-1} \cdot B_i^{-1} \cdot S_i, \quad (1)$$

where B_i is a temperature factor which accounts for the intensity contribution of excited vibrational states, and is represented by the Boltzmann distribution

$$B_i = 1 - \exp\left(-\frac{hv_i c}{kT}\right). \quad (2)$$

In equation (1) v_0 is the frequency of the laser excitation line (in this work, we have used the excitation frequency $v_0 = 9398.5 \text{ cm}^{-1}$, which corresponds to the wavelength of 1064 nm of a Nd:YAG laser), v_i is the frequency of normal mode (cm^{-1}), while S_i is the Raman scattering activity of the normal mode Q_i . I_i^R is given in arbitrary units (C is a constant equal 10^{-12}). In Equation (2) h , k , c , and T are the Planck constant, Boltzmann constant, light-speed and temperature (in Kelvin), respectively. The B_i factor was assumed to 1, otherwise, the calculated Raman intensities for the bands below 300 cm^{-1} were extremely overestimated, in comparison to experiment [21].

In aromatic compounds, C-H stretching frequencies appear in the range of $3000\text{--}3100 \text{ cm}^{-1}$; in-plane C-H bending vibrations appear in the range of $1000\text{--}1300 \text{ cm}^{-1}$; and out-of-plane C-H bending vibrations appear in the range $750\text{--}1000 \text{ cm}^{-1}$. In the flavone, the C-H stretching vibrations are predicted at $3098\text{--}3151 \text{ cm}^{-1}$ for B3LYP/6-311++G(d,p) level of theory. These vibrations are observed experimentally in the range of $3040\text{--}3100 \text{ cm}^{-1}$ in the infrared spectra. Four C-H stretching modes of the phenyl group (ν_{66} , ν_{68} , ν_{70} , ν_{75}) are predicted in this region. These vibrations are observed at 3040 cm^{-1} and 3070 cm^{-1} in the infrared spectra. In the high frequency region, the TED calculations show that all the C-H stretching vibrations are pure modes. In-plane C-H bending vibrations are observed in the range of $1079\text{--}1260 \text{ cm}^{-1}$ for infrared spectra. In-plane C-H bending vibrations of flavone molecule observed at 1079 cm^{-1} , 1001 cm^{-1} , 1129 cm^{-1} and 1260 cm^{-1} in the infrared spectra. Out-of-plane C-H bending vibrations are observed at 769 cm^{-1} , 851 cm^{-1} , 868 cm^{-1} , 906 cm^{-1} and 925 cm^{-1} for flavone. The theoretical wave number of (in-plane and out-of-plane) C-H stretching coincides very well with experimental values.

The most intensive peak is C=O stretching and is observed at 1646 cm^{-1} in IR, and 1633 cm^{-1} in RA for flavone. Fundamental CC=O bending mode was at 606 cm^{-1} (IR), 616 cm^{-1} (RA) for flavone. This peak calculated at 599 cm^{-1} for B3LYP/6-311++G(d,p) level of theory for flavone. The CC ring stretching vibrations for all rings assigned to 1606 cm^{-1} in the flavone. CC stretching modes for all rings observed between $1569 \text{ cm}^{-1}\text{--}1011 \text{ cm}^{-1}$ for flavone, where they are expected to be.

Table 3. Comparison of the observed and calculated vibrational spectra of flavone.

V _i	B3LYP/6-311++G(d,p)			B3LYP/6-31++G(d,p)			Ra [5]	SERS [5]	Gas phase [6]	Exp. IR.	Exp. RA	TED ^s (%)
	Freq. ^a	Freq. ^b	IR. ^c	RA. ^d	Freq. ^a	Freq. ^c						
V ₁	34	33	0.09	0.06	33	32	-	-	-	-	-	Γ _{cccc} (50) Γ _{cccc} (42)
V ₂	57	56	0.07	4.85	58	57	-	-	-	-	-	Γ _{cccc} (39) Γ _{cooc} (27)
V ₃	102	100	0.07	0.10	103	100	-	-	-	94 m	-	δ _{ccc} (33) δ _{cco} (20)
V ₄	119	116	0.52	0.10	122	119	-	-	-	123 w	-	Γ _{cccc} (36) Γ _{cccc} (28)
V ₅	154	151	0.08	0.46	157	153	-	-	-	144 w	-	Γ _{cccc} (33) Γ _{cooc} (25)
V ₆	202	198	0.30	0.02	205	200	-	-	-	215 m	-	Γ _{cccc} (33) Γ _{cccc} (30)
V ₇	264	258	0.29	0.34	264	258	-	-	-	-	-	δ _{ccc} (23) ν _{cc} (16) δ _{cco} (15) ν _{co} (10)
V ₈	281	275	0.01	63.69	283	276	-	-	-	267 w	-	Γ _{cccc} (13) ν _{cc} (10)
V ₉	294	288	0.60	24.56	294	288	295	346	-	294 w	-	δ _{ccc} (25) δ _{cco} (16)
V ₁₀	347	339	0.97	0.78	347	339	-	-	-	-	-	δ _{ccc} (35) δ _{cco} (24)
V ₁₁	410	401	0.03	13.01	412	403	-	-	-	-	-	Γ _{cccc} (65) Γ _{cccc} (34) (P)
V ₁₂	434	425	0.06	2.24	436	426	-	-	-	-	-	Γ _{cccc} (43) Γ _{cccc} (19)
V ₁₃	468	458	0.77	3.58	469	459	-	-	-	454 vw	-	Γ _{cccc} (30) Γ _{cccc} (21) (P)
V ₁₄	504	493	0.52	3.57	503	492	-	-	-	-	-	δ _{ccc} (32) δ _{ccc} (10) δ _{cco} (13) δ _{coo} (12)
V ₁₅	514	503	0.46	1.49	514	503	501	-	-	498 vw	-	δ _{ccc} (25) ν _{cc} (22) δ _{cco} (18)
V ₁₆	535	523	0.96	3.61	538	526	511	520	-	510 m	-	Γ _{cccc} (25) Γ _{cccc} (25) Γ _{cccc} (15)
V ₁₇	588	575	0.15	17.53	586	573	-	-	-	529 w	-	δ _{ccc} (28) δ _{ccc} (14)
V ₁₈	613	599	2.76	35.24	612	598	-	-	-	-	-	δ _{cco} (32) δ _{ccc} (14)
V ₁₉	633	619	0.04	41.74	631	617	621	614	-	606 m	-	δ _{ccc} (58) (P) δ _{ccc} (20)
V ₂₀	663	649	0.32	65.82	663	648	652	-	-	650 w	-	Γ _{cccc} (13) Γ _{cccc} (13) Γ _{cooc} (11) Γ _{cccc} (11) (P)
V ₂₁	685	670	2.47	20.36	684	669	675	680	-	649 vw	-	Γ _{cccc} (24) Γ _{cccc} (18)
V ₂₂	686	671	0.83	0.21	684	669	-	-	-	673 m	-	δ _{ccc} (15) (P)
V ₂₃	703	687	6.26	7.45	702	686	-	-	-	687 m	-	Γ _{cccc} (55) Γ _{cccc} (33) (P)
V ₂₄	754	737	0.88	3.75	755	738	-	-	-	-	-	δ _{ccc} (41) δ _{ccc} (12)
V ₂₅	768	751	3.26	33.53	765	748	-	-	-	-	-	Γ _{cccc} (33) Γ _{cccc} (24) Γ _{cccc} (16)
V ₂₆	783	766	17.36	5.80	783	766	746	755	-	745	-	Γ _{cccc} (38) Γ _{cccc} (15) (P)
V ₂₇	789	772	0.55	2.17	788	771	-	-	-	769 s	-	Γ _{cccc} (22) Γ _{cccc} (19)
V ₂₈	853	835	0.43	4.02	855	837	-	-	-	-	-	Γ _{cccc} (93) (P)
V ₂₉	860	841	2.02	5.89	860	841	-	-	-	-	-	δ _{ccc} (28) ν _{oc} (15) (P)
V ₃₀	873	854	3.35	50.73	874	855	856	838	-	850 vw	-	Γ _{cccc} (41) Γ _{cccc} (33)
V ₃₁	882	862	0.50	1.62	884	864	-	-	-	-	-	Γ _{cccc} (45) Γ _{cccc} (17) Γ _{cccc} (17)
V ₃₂	920	900	3.54	65.77	919	899	-	-	-	868 w	-	δ _{ccc} (15) δ _{ccc} (12) δ _{ccc} (10) ν _{oc} (11) ν _{cc} (10) (P)
V ₃₃	942	921	0.30	69.54	942	921	-	-	-	906 m	-	Γ _{cccc} (57) Γ _{cccc} (32) (P)
V ₃₄	979	957	0.26	100	979	957	929	-	-	925 vw	-	Γ _{cccc} (48) Γ _{cccc} (37)
V ₃₅	991	969	0.08	48.29	989	967	-	-	-	-	-	Γ _{cccc} (53) (P) Γ _{cccc} (33) (P)
V ₃₆	1003	981	0.03	0.95	1005	983	-	-	-	-	-	Γ _{cccc} (60) Γ _{cccc} (29)
V ₃₇	1008	986	0.02	1.37	1008	986	-	-	-	-	-	Γ _{cccc} (77) (P)
V ₃₈	1016	993	0.32	2.73	1014	992	-	-	-	-	-	ν _{cc} (40) (P) δ _{ccc} (40) (P)
V ₃₉	1031	1009	1.50	2.84	1035	1013	-	-	-	-	-	ν _{cc} (46) ν _{oc} (17) (P)

Table 3. Continued

	B3LYP/6-311++G(d,p)				B3LYP/6-31++G(d,p)				Exp. IR.	Exp. RA	TED ^c (%)
	Freq. ^a	Freq. ^b	IR. ^c	RA. ^d	Freq. ^a	Freq. ^b	SERS [5]	Gas phase [6]			
ν_{40}	1049	1026	3.27	3.03	1052	1029	1002	1005	1011 w	1000 s	ν_{CC} (33) (P) ν_{CC} (20) δ_{CCH} (15) (P)
ν_{41}	1063	1040	3.07	3.20	1067	1044	1013		1029 m	1012 m	ν_{OC} (20) ν_{CC} (19) (P)
ν_{42}	1108	1084	1.87	0.65	1110	1086	1048		1044 m	1044 vw	ν_{CC} (36) δ_{CCH} (27) (P)
ν_{43}	1109	1085	0.05	5.70	1111	1086					δ_{CCH} (35) ν_{CC} (19)
ν_{44}	1147	1122	7.98	1.89	1149	1124		1098	1079 w		δ_{CCH} (44) ν_{CC} (37)
ν_{45}	1174	1148	0.03	1.73	1177	1151					δ_{CCH} (71) ν_{CC} (16)
ν_{46}	1186	1160	0.03	0.06	1188	1162	1100		1101 m	1100 vw	δ_{CCH} (74) (P) ν_{CC} (15) (P)
ν_{47}	1208	1182	2.22	4.85	1211	1184	1143		1129 s	1131 vw	δ_{CCH} (75) (P) ν_{CC} (15) (P)
ν_{48}	1235	1208	7.24	0.08	1246	1219	1162	1170	-	1160 vw	ν_{OC} (39) ν_{CC} (27) δ_{CCH} (15)
ν_{49}	1253	1225	0.60	0.10	1257	1230	1195		-	1191 w	δ_{CCH} (28) ν_{CC} (22) (P) ν_{CC} (R-P) (18)
ν_{50}	1273	1245	4.44	0.46	1278	1250	1235	1244	1226 m	1235 s	δ_{CCH} (47) ν_{CC} (12) (P)
ν_{51}	1307	1278	1.00	0.02	1313	1284	1270	1256	1260 m	1266 s	δ_{CCH} (29) ν_{CC} (26) (P)
ν_{52}	1330	1301	10.06	0.34	1339	1310			1283 w		ν_{CC} (44) (P)
ν_{53}	1355	1325	3.02	63.69	1365	1335			-		ν_{CC} (31) ν_{CC} (24) (P) δ_{CCH} (25) (P)
ν_{54}	1359	1329	0.76	24.56	1372	1342	1336	1322	1311 w	1334 m	ν_{CC} (45) δ_{CCH} (28) (P)
ν_{55}	1386	1356	65.23	0.78	1397	1366	1377	1359	1376 s	1374 w	ν_{CC} (21) ν_{CC} (18) δ_{CCH} (11)
ν_{56}	1478	1445	3.93	13.01	1483	1450			-		δ_{CCH} (52) ν_{CC} (29)
ν_{57}	1492	1459	19.66	2.24	1498	1465			-		δ_{CCH} (39) ν_{CC} (28)
ν_{58}	1501	1468	0.63	3.58	1507	1474	1452	1403	1449 m	1449 w	δ_{CCH} (51) ν_{CC} (35)
ν_{59}	1525	1491	2.77	3.57	1531	1497	1470	1474	1466 s	1469 w	δ_{CCH} (60) (P) ν_{CC} (29)
ν_{60}	1604	1568	8.84	1.49	1612	1576		1495	1495 s		ν_{CC} (64)
ν_{61}	1616	1580	0.81	3.61	1624	1588	1570	1556	1569 m	1571 s	ν_{CC} (48) (P) ν_{CC} (19) (P)
ν_{62}	1642	1606	0.07	17.53	1650	1614			-		ν_{CC} (60) (P) δ_{CCH} (15)
ν_{63}	1643	1607	11.42	35.24	1651	1615			-		ν_{CC} (59)
ν_{64}	1654	1618	18.50	41.74	1662	1626	1603	1603	1606 m	1602 s	ν_{CC} (64)
ν_{65}	1704	1666	100	65.82	1712	1675	1634	1636	1646 vs	1633 vs	ν_{CO} (77)
ν_{66}	3168	3098	0.08	20.36	3185	3115		3025	3040 vw		ν_{CH} (99) (P)
ν_{67}	3173	3103	0.54	0.21	3191	3121			3059 s		ν_{CH} (100)
ν_{68}	3178	3108	1.28	7.45	3195	3125	3075	2929	3070 vw	3069 s	ν_{CH} (97) (P)
ν_{69}	3186	3116	1.51	3.75	3204	3134			-		ν_{CH} (98)
ν_{70}	3188	3118	3.31	33.53	3205	3135			-		ν_{CH} (97) (P)
ν_{71}	3197	3126	1.66	5.80	3214	3144			-		ν_{CH} (94)
ν_{72}	3198	3127	0.62	2.17	3216	3145			-		ν_{CH} (99)
ν_{73}	3202	3131	1.83	4.02	3219	3149			-		ν_{CH} (99)
ν_{74}	3209	3139	0.62	5.89	3226	3155			-		ν_{CH} (98) (P)
ν_{75}	3222	3151	0.22	50.73	3242	3171		3095	3100 vw	3135 vw	ν_{CH} (97)

P: Phenyl (C-Ring); R: A and B Rings; ν : Stretching; δ : Bending; Γ : Torsion; vs: Very strong; s: Strong; m: Medium; w: Weak; vw: Very weak^a Unscaled frequencies; ^b Scaling factor 0.8900; ^c Scaling factor 0.9781; Only contributions $\geq 10\%$ are listed.^d Relative absorption intensities normalized with highest peak absorption equal to 100^e Relative Raman intensities calculated by Eq. 1 and normalized to 100^f Total energy distribution calculated B3LYP/6-311++G(d,p) level.

5. Conclusion

The IR spectrum of the title compound was computed using the B3LYP methods in conjunction with the 6-31++G(d,p) and 6-311++G(d,p) basis sets. Results are in good agreement with the observed FT-IR spectrum. The scale factors were used in order to compare how the calculated wave numbers are consistent with those of the experimental values.

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