

Vibrational spectroscopic studies and ab initio calculations of 5-methyl-2-(*p*-fluorophenyl)benzoxazole

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Abstract

FT-Raman and FT-IR spectra of 5-methyl-2-(*p*-fluorophenyl)benzoxazole were recorded and analysed. The vibrational frequencies of the compound have been computed using the Hartree-Fock/6-31G* basis and compared with the experimental values.

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1. Introduction

Benzoxazole derivatives are the structural isoesters of naturally occurring nucleotides such as adenine and guanine, which allows them to interact easily with the biopolymers of living systems and different kinds of biological activity have been obtained [1–5]. Besides, due to their kind of action, it has been reported that they have shown low toxicity in warm-blooded animals [4,6]. Synthesis and microbiological activity of 5-substituted-2-(*p*-substitutedphenyl)benzoxazole derivatives are reported by Yalcin et al. [7–10]. Ab initio quantum mechanical method is at present widely used for simulating IR spectrum. Such simulations are indispensable tools to perform normal coordinate analysis so that modern vibrational spectroscopy is unimaginable without involving them. In the present study the FT-IR, FT-Raman and theoretical calculations of the wavenumbers of the title compound are reported.

2. Experimental

For the synthesis of the benzoxazole derivative, using aqueous mineral acids as the condensation reagent did not provide

successful results, because of the oxazole ring which was easily hydrolysed under these conditions [11]. Reactions which occurred in pyridine or xylene also has low yields. Finally, polyphosphoric acid was chosen as the reagent for cyclodehydration in the synthesis of the title compound as it has good solvent power and contains anhydride group which combine with the water formed in the reaction centre in order to prevent effective acidity. The stability of the oxazole ring increases under these conditions and high temperature could be used [11]. The title compound was prepared by heating 2-hydroxy-5-methyl aniline with the appropriate carboxylic acid in polyphosphoric acid [11] and the structure of the title compound were supported by elemental analysis and spectral data by Yalcin et al. [11]. The FT-IR spectrum (Fig. 1) was recorded using a Perkin-Elmer FT-IR 1760× spectrometer. The spectral resolution was 4 cm⁻¹. Standard KBr technique with 1 mg sample per 300 mg KBr was used. The FT-Raman spectrum (Fig. 2) was obtained on a Bruker IFS 66 V NIR-FT instrument equipped with a FRA106 Raman module. A Nd/YAG laser at 1064 nm with an output on 300 mW was used as the exciting source. The detector was a Ge-diode cooled to liquid nitrogen temperature. One thousand scans were accumulated with a total registration time of about 30 min. The spectral resolution after apodization was 6 cm⁻¹. A correction according to the fourth power scattering factor was performed, but no correction to instrumental response was done.

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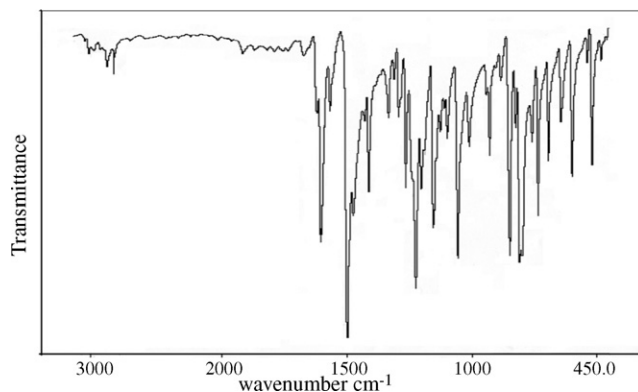


Fig. 1. FT-IR spectrum of 5-methyl-2-(*p*-fluorophenyl)benzoxazole.

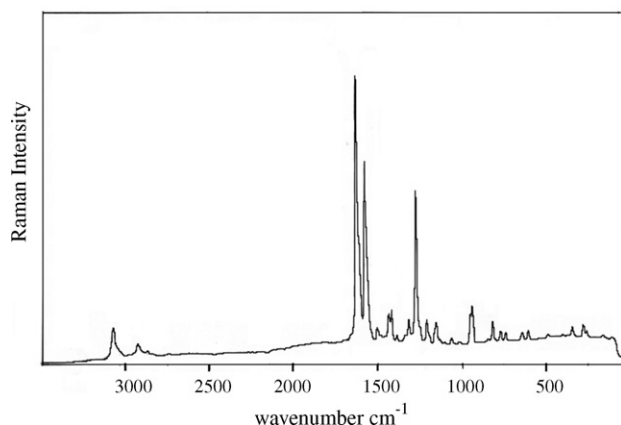


Fig. 2. FT-Raman spectrum of 5-methyl-2-(*p*-fluorophenyl)benzoxazole.

3. Computational details

Calculations of the title compound were carried out with Gaussian03 program [12] using the HF/6-31G* basis set to predict the molecular structure and vibrational wavenumbers. Molecular geometry was fully optimized by Berny's optimization algorithm using redundant internal coordinates. Harmonic vibrational wavenumbers were calculated using the analytic second derivatives to confirm the convergence to minima on the potential surface. The wavenumber values computed at the Hartree–Fock level contain known systematic errors due to the negligence of electron correlation [13]. We therefore, have used the scaling factor value of 0.8929 for HF/6-31G* basis set. Parameters corresponding to optimized geometry of the title compound (Fig. 3) are given in Table 1. The absence of

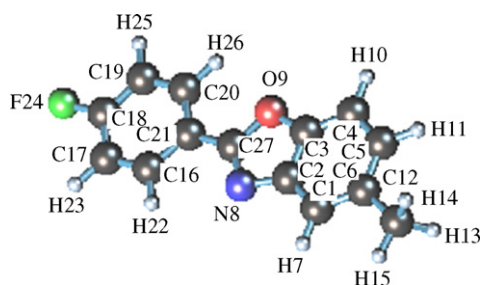


Fig. 3. Optimized geometry of 5-methyl-2-(*p*-fluorophenyl)benzoxazole.

imaginary wavenumbers on the calculated vibrational spectrum confirms that the structure deduced corresponds to minimum energy. In total there are 75 vibrations from 3050 to 38 cm^{-1} . The assignments of the calculated wavenumbers are aided by the animation option of MOLEKEL program, which gives a visual presentation of the vibrational modes [14,15].

4. Results and discussion

The observed Raman and IR bands with their relative intensities and calculated wavenumbers and assignments are given in Table 2. In aromatic compounds the asymmetric stretching vibrations of CH_3 are expected in the range 2905–3000 cm^{-1} and symmetric CH_3 vibrations in the range 2860–2870 cm^{-1} [16,17]. The first of these results from the asymmetric stretching $\nu_a\text{CH}_3$ mode in which two C–H bonds of the methyl group are extending while the third one is contracting. The second arises from symmetrical stretching $\nu_s\text{CH}_3$ in which all three of the C–H bonds extend and contract in phase. The asymmetric stretching modes of the methyl group are calculated to be 2931, 2907 cm^{-1} and the symmetric mode at 2861 cm^{-1} . $\nu_a\text{CH}_3$ vibrations are observed at 2921 (IR), 2928 cm^{-1} (Raman) and $\nu_s\text{CH}_3$ at $\sim 2875 \text{ cm}^{-1}$ in both spectra. Two bending can occur within a methyl group. The first of these, the symmetrical bending vibration, involves the in-phase bending of the C–H bonds. The second, the asymmetrical bending vibration, involves out-of-phase bending of the C–H bonds. The asymmetric deformations are expected in the range 1400–1485 cm^{-1} [16]. The calculated values of $\delta_a\text{CH}_3$ modes are at 1469 and 1457 cm^{-1} . Experimentally no bands are observed. In many molecules the symmetric deformation $\delta_s\text{CH}_3$ appears with an intensity varying from medium to strong and expected in the range $1380 \pm 25 \text{ cm}^{-1}$ [16]. The band at 1391 cm^{-1} in the Raman spectrum and at 1400 cm^{-1} (calculated) are assigned to $\delta_s\text{CH}_3$. Aromatic molecules display a methyl rock in the neighbourhood of 1045 cm^{-1} [16]. The second rock in the region $970 \pm 70 \text{ cm}^{-1}$ [16] is more difficult to find among the C–H out-of-plane deformations. For the title compound, these modes are calculated at 1048 and 989 cm^{-1} and only one band is observed at 1053 cm^{-1} in the IR spectrum. The torsional modes of CH_3 are seen in the range 38–481 cm^{-1} [16].

Fluorine atoms directly attached to an aromatic ring give rise to bands in the region 1270–1100 cm^{-1} [17]. Many of these compounds including the simpler ones with one fluorine only on the ring absorb near 1230 cm^{-1} [17]. Saxena et al. [18] reported a value 1157 cm^{-1} for $\nu\text{C–F}$ stretching mode for polybenzodithiazole. For the title compound the stretching mode $\nu\text{C–F}$ is observed in the IR spectrum at 1223 cm^{-1} and the calculated value is 1244 cm^{-1} .

The C=N stretching skeletal bands are observed in the range 1672–1566 cm^{-1} [11,18–20]. Saxena et al. [18] reported a value 1608 cm^{-1} for polybenzodithiazole and Klots and Collier [21] reported a value 1517 cm^{-1} for benzoxazole as $\nu\text{C=N}$ stretching mode. The bands at 1661 cm^{-1} in the Raman spectrum, 1671 cm^{-1} in the IR spectrum and 1643 cm^{-1} given by calculation are assigned as $\nu\text{C=N}$.

Table 1
Optimized geometrical parameters of 5-methyl-2-(*p*-fluorophenyl)benzoxazole, atom labeling is according to Fig. 3

Bond length (Å)		Bond angle (°)		Dihedral angle (°)	
C ₁ –C ₂	1.3884	A(2,1,6)	118.2	D(6,1,2,3)	–0.001
C ₁ –C ₆	1.385	A(2,1,7)	120.4	D(6,1,2,8)	–179.99
C ₁ –H ₇	1.0744	A(6,1,7)	121.4	D(7,1,2,3)	179.99
C ₂ –C ₃	1.3776	A(1,2,3)	120.2	D(7,1,2,8)	0.004
C ₂ –N ₈	1.3903	A(1,2,8)	131.5	D(2,1,6,5)	0.008
C ₃ –C ₄	1.3777	A(3,2,8)	108.2	D(2,1,6,12)	–179.94
C ₃ –O ₉	1.3594	A(2,3,4)	123.4	D(7,1,6,5)	–179.98
C ₄ –C ₅	1.3828	A(2,3,9)	107.2	D(7,1,6,12)	0.065
C ₄ –H ₁₀	1.0737	A(4,3,9)	129.4	D(1,2,3,4)	–0.005
C ₅ –C ₆	1.4047	A(3,4,5)	115.8	D(1,2,3,9)	–179.99
C ₅ –H ₁₁	1.076	A(3,4,10)	122.1	D(8,2,3,4)	179.98
C ₆ –C ₁₂	1.5126	A(5,4,10)	122.1	D(8,2,3,9)	–0.003
N ₈ –C ₂₇	1.2727	A(4,5,6)	122.5	D(1,2,8,27)	179.99
O ₉ –H ₂₆	2.4689	A(4,5,11)	118.8	D(3,2,8,27)	0.002
O ₉ –C ₂₇	1.347	A(6,5,11)	118.7	D(2,3,4,5)	0.003
C ₁₂ –H ₁₃	1.0859	A(1,6,5)	119.8	D(2,3,4,10)	–179.99
C ₁₂ –H ₁₄	1.0858	A(1,6,12)	120.8	D(9,3,4,5)	179.99
C ₁₂ –H ₁₅	1.0835	A(5,6,12)	119.4	D(9,3,4,10)	–0.002
C ₁₆ –C ₁₇	1.3802	A(2,8,27)	104.5	D(2,3,9,26)	179.77
C ₁₆ –C ₂₁	1.3931	A(3,9,26)	170.6	D(2,3,9,27)	0.002
C ₁₆ –H ₂₂	1.0731	A(3,9,27)	104.6	D(4,3,9,26)	–0.21
C ₁₇ –C ₁₈	1.3808	A(26,9,27)	84.8	D(4,3,9,27)	–179.98
C ₁₇ –H ₂₃	1.0734	A(6,12,13)	111.2	D(3,4,5,6)	0.005
C ₁₈ –C ₁₉	1.3778	A(6,12,14)	111.2	D(3,4,5,11)	–179.99
C ₁₈ –F ₂₄	1.3267	A(6,12,15)	111.2	D(10,4,5,6)	179.99
C ₁₉ –C ₂₀	1.3836	A(13,12,14)	107.5	D(10,4,5,11)	–0.002
C ₁₉ –H ₂₅	1.0734	A(13,12,15)	107.8	D(4,5,6,1)	–0.011
C ₂₀ –C ₂₁	1.3902	A(14,12,15)	107.8	D(4,5,6,12)	179.94
C ₂₀ –H ₂₆	1.073	A(17,16,21)	120.4	D(11,5,6,1)	179.98
C ₂₁ –C ₂₇	1.4667	A(17,16,22)	120.4	D(11,5,6,12)	–0.06
		A(21,16,22)	119.2	D(1,6,12,13)	119.34
		A(16,17,18)	118.6	D(1,6,12,14)	–120.95
		A(16,17,23)	121.7	D(1,6,12,15)	–0.79
		A(18,17,23)	119.7	D(5,6,12,13)	–60.61
		A(17,18,19)	122.4	D(5,6,12,14)	59.10
		A(17,18,24)	118.8	D(5,6,12,15)	179.25
		A(19,18,24)	118.9	D(2,8,27,9)	–0.0004
		A(18,19,20)	118.6	D(2,8,27,21)	–178.00
		A(18,19,25)	119.8	D(3,9,26,20)	–179.82
		A(20,19,25)	121.7	D(27,9,26,20)	–0.04
		A(19,20,21)	120.4	D(3,9,27,8)	–0.00
		A(19,20,26)	119.7	D(3,9,27,21)	178.00
		A(21,20,26)	119.9	D(26,9,27,8)	–179.96
		A(16,21,20)	119.6	D(26,9,27,21)	0.03
		A(16,21,27)	119.3	D(21,16,17,18)	–0.004
		A(20,21,27)	121.1	D(21,16,17,23)	178.00
		A(9,26,20)	96.8	D(22,16,17,18)	180.00
		A(8,27,9)	115.4	D(22,16,17,23)	–0.0005
		A(8,27,21)	127.2	D(17,16,21,20)	0.00
		A(9,27,21)	117.4	D(17,16,21,27)	180.00
				D(22,16,21,20)	–180.00
				D(22,16,21,27)	–0.001
				D(16,17,18,19)	0.001
				D(16,17,18,24)	180.00
				D(23,17,18,19)	–180.00
				D(23,17,18,24)	–0.004
				D(17,18,19,20)	0.001
				D(17,18,19,25)	180.00
				D(24,18,19,20)	–179.99
				D(24,18,19,25)	0.01
				D(18,19,20,21)	–0.001
				D(18,19,20,26)	–179.99
				D(25,19,20,21)	180.00
				D(25,19,20,26)	0.007

Table 1 (Continued)

Bond length (Å)	Bond angle (°)	Dihedral angle (°)
		<i>D</i> (19,20,21,16)
		–0.002
		<i>D</i> (19,20,21,27)
		–180.00
		<i>D</i> (26,20,21,16)
		179.99
		<i>D</i> (26,20,21,27)
		–0.006
		<i>D</i> (19,20,26,9)
		–179.98
		<i>D</i> (21,20,26,9)
		0.02
		<i>D</i> (16,21,27,8)
		–0.03
		<i>D</i> (16,21,27,9)
		179.96
		<i>D</i> (20,21,27,8)
		179.96
		<i>D</i> (20,21,27,9)
		–0.04

Since the identification of all the normal modes of vibrations of large molecules is not trivial, we tried to simplify the problem by considering each molecule as a substituted benzene. Such an idea has already been successfully utilized by several workers for the vibrational assignments of molecules containing multiple homo- and heteroaromatic rings [22–26]. In the following discussion, the phenyl rings attached with methyl group and fluorine are designated as rings I and II, respectively. The modes in the two phenyl rings will differ in wavenumber and the magnitude of splitting will depend on the strength of interactions between different parts (internal coordinates) of the two rings. For some modes, this splitting is so small that they may be considered as quasi-degenerate and for the other modes a significant amount of splitting is observed. Such observations have already been reported [22–24,27].

The benzoxazole ring stretching vibrations exist in the range 1504–1309 cm^{-1} in both spectra [18,28]. Bands observed at 1504, 1433, 1418 cm^{-1} in the Raman spectrum [18] and 1499, 1474, 1412 and 1309 cm^{-1} in the IR spectrum are assigned as the ring stretching vibrations. Klots and Collier [21] reported the bands at 1615, 1604, 1475 and 1451 cm^{-1} as fundamental ring vibrations of the benzoxazole ring.

As expected the asymmetric C–O–C vibration produce strong band at 1263 and 1269 cm^{-1} in the IR and Raman spectrum, respectively [11,19]. The symmetric C–O–C stretching vibration appear as a weak band at 1055 cm^{-1} in the IR spectrum and at 1061 cm^{-1} in the Raman spectrum [11,19]. The ab initio calculations give 1261 and 1060 cm^{-1} as asymmetric and symmetric C–O–C modes, respectively. The C–O–C stretching is reported at 1250 and 1073 cm^{-1} for 2-mercaptobenzoxazole [29].

Primary aromatic amines with nitrogen directly on the ring absorb strongly at 1330–1260 cm^{-1} due to stretching of the phenyl carbon–nitrogen bond [17]. For 2-mercaptobenzoxazole this mode [29] is reported at 1340 cm^{-1} (Raman) and 1325 cm^{-1} (ab initio calculations). Sandhyarani et al. [30] reported νCN at $\sim 1318 \text{ cm}^{-1}$ for 2-mercaptobenzothiazole. We have observed this mode at 1332 cm^{-1} in IR spectrum, 1315 cm^{-1} in Raman spectrum and 1315 cm^{-1} theoretically.

The existence of one or more aromatic rings in a structure is normally readily determined from the C–H and C=C–C ring related vibrations. The C–H stretching occurs above 3000 cm^{-1} and is typically exhibited as a multiplicity of weak to moderate bands, compared with the aliphatic C–H stretch [31]. Klot

and Collier [21] reported the bands at 3085, 3074, 3065 and 3045 cm^{-1} as $\nu\text{C–H}$ modes for benzoxazole. In the present case, ab initio calculations give $\nu\text{C–H}$ modes in the range 3001–3050 cm^{-1} . The bands observed at 3023, 3048 cm^{-1} in the IR spectrum and at 3036, 3075 cm^{-1} in the Raman spectrum are assigned as these modes

For the *para*-substituted light–heavy, fluorine attached phenyl ring the νPh modes are expected in the range 1280–1620 cm^{-1} and for the trisubstituted benzene ring these modes are seen in the region 1250–1610 cm^{-1} [16]. For *para*-substituted benzenes, the δCH modes are seen in the range 995–1315 cm^{-1} [16] and for trisubstituted benzenes these modes are in the range 1050–1280 cm^{-1} [16]. Bands observed at 1009, 1096, 1125, 1153, 1201, 1291, 1309 cm^{-1} in the IR spectrum and at 1154, 1208 cm^{-1} in the Raman spectrum are assigned as δCH modes.

The C–H out-of-plane deformations are observed between 1000 and 700 cm^{-1} [16]. Generally the C–H out-of-plane deformations with the highest wavenumbers have a weaker intensity than those absorbing at lower wavenumbers. These γCH modes are observed at 847, 882 cm^{-1} in the IR spectrum. The ab initio calculations give these modes at 817, 834, 856, 895, 958, 973 and 993 cm^{-1} . For benzoxazole, Klots and Collier [21] reported the bands at 932, 847 and 746 cm^{-1} as out-of-plane deformations of the benzene ring. According to Collier and Klots [32] the non-planar vibrations are observed at 970, 932, 864, 847, 764, 746, 620, 574, 417, 254, 218 cm^{-1} for benzoxazole and at 973, 939, 856, 824, 757, 729, 584, 489, 419, 207, 192 cm^{-1} for benzothiazole. The planar modes below 1000 cm^{-1} for benzoxazole are reported to be at 920, 870, 778, 622, 538, 413 cm^{-1} and for benzothiazole at 873, 801, 712, 666, 531, 504, 350 cm^{-1} [32]. We have also observed the planar and non-planar modes for the title compound in this region. Two very strong CH out-of-plane deformation bands, occurring at $840 \pm 50 \text{ cm}^{-1}$ is typical for 1,4-disubstituted benzene [16]. For the title compound, a very strong γCH band is observed at 847 cm^{-1} . Again, according to literature [16,17] a lower γCH absorbs in the neighbourhood $820 \pm 45 \text{ cm}^{-1}$, but is much weaker or infrared inactive. The ab initio calculation gives a γCH at 834 cm^{-1} and no band is experimentally observed for this mode. In the case of trisubstituted benzenes, two γCH bands are observed at 890 ± 50 and $815 \pm 45 \text{ cm}^{-1}$ [16]. We have observed bands at 882 cm^{-1} in the IR spectrum and at 816 cm^{-1} in the Raman spectrum. Theoretically the values obtained are 895 and 817 cm^{-1} .

Table 2
Calculated vibrational wavenumbers, measured infrared and Raman band positions and assignments for 5-methyl-2-(*p*-fluorophenyl)benzoxazole

$\nu_{\text{calculated}}$ (cm ⁻¹)	ν_{IR} (cm ⁻¹)	ν_{Raman} (cm ⁻¹)	Assignments
3050		3075 m	$\nu(\text{CH})\text{II}$
3049	3048 w		$\nu(\text{CH})\text{II}$
3036		3036 vw	$\nu(\text{CH})\text{I}$
3035			$\nu(\text{CH})\text{II}$
3034			$\nu(\text{CH})\text{II}$
3025	3023 w		$\nu(\text{CH})\text{I}$
3001			$\nu(\text{CH})\text{I}$
2931	2921 w	2928 w	$\nu_{\text{a}}\text{CH}_3$
2907			$\nu_{\text{a}}\text{CH}_3$
2861	2873 w	2875 vw	$\nu_{\text{s}}\text{CH}_3$
1643	1671 wbr	1661 vw	$\nu\text{C}=\text{N}$
1623	1617 m	1624 vvs	$\nu\text{Ph II}$
1611			$\nu\text{Ph I}$
1605	1603 s		$\nu\text{Ph I, II}$
1585	1566 m	1572 s	$\nu\text{Ph II}$
1511	1499 vvs	1504 w	$\nu\text{Ph I}$
1482	1474 s		$\nu\text{Ph I}$
1469			$\delta_{\text{a}}\text{CH}_3$
1457			$\delta_{\text{a}}\text{CH}_3$
1423		1433 m	$\nu\text{Ph I}$
1404	1412 s	1418 m	$\nu\text{Ph I, II}$
1400		1391 vw	$\delta_{\text{s}}\text{CH}_3$
1315	1332 m	1315 w	$\nu\text{C}-\text{N}$
1286	1309 w		$\nu\text{Ph II}$
1273	1291 m		$\nu\text{CH I}$
1261	1263 s	1269 s	$\nu_{\text{a}}\text{C}-\text{O}-\text{C}$
1244	1223 vs		$\nu\text{C}-\text{F}$
1199	1201 s	1208 w	$\delta\text{CH I}$
1189			$\delta\text{CH I}$
1161	1153 s	1154 w	$\delta\text{CH II}$
1143			$\delta\text{CH II}$
1122	1125 m		$\delta\text{CH I}$
1097	1096 m		$\delta\text{CH I}$
1066			$\delta\text{CH II}$
1060	1055 vs	1061 vw	$\nu_{\text{s}}\text{C}-\text{O}-\text{C}$
1048	1053 w		ρCH_3
994	1009 m		$\delta\text{CH II}$
993			$\gamma\text{CH II}$
989			ρCH_3
973			$\gamma\text{CH II}$
958	950 w	948 wsh	$\gamma\text{CH I}$
926	927 m	936 m	δNCO
919			$\delta\text{Ph(X)I}$
895	882 w		$\gamma\text{CH I}$
856	847 vs		$\gamma\text{CH II}$
834			$\gamma\text{CH II}$
819	823 m		$\delta\text{Ph I, II}$
817		816 w	$\gamma\text{CH I}$
795	809 vs		$\delta\text{Ph I}$
752	757 m	768 w	$\gamma\text{Ph I}$
742	734 s	740 w	$\gamma\text{Ph I, II}$
742			$\delta\text{Ph I}$
689	692 m		$\gamma\text{Ph II}$
626	642 m	640 w	$\delta\text{Ph I, II}$
621			$\delta\text{Ph II}$
594	597 s	605 w	$\gamma\text{Ph(X) I}$
578			$\delta\text{Ph I, II}$
524	536 w		$\delta\text{Ph I, II}$
519	517 s		$\gamma\text{Ph II}$
466	481 w		$\delta\text{Ph I, II}$
437			$\gamma\text{Ph I}$
414			$\gamma\text{Ph II}$
412			$\delta\text{Ph II}$

Table 2 (Continued)

$\nu_{\text{calculated}}$ (cm ⁻¹)	ν_{IR} (cm ⁻¹)	ν_{Raman} (cm ⁻¹)	Assignments
388			$\gamma\text{Ph I}$
347		343 w	$\delta\text{Ph I, II}$, τCH_3
324			$\gamma\text{Ph I, II}$, τCH_3
260		277 w	$\gamma\text{Ph(X) I}$
253			$\tau\text{Ph II}$, τCH_3
235			τCH_3
186			$\tau\text{Ph I, II}$, τCH_3
120			$\tau\text{Ph I, II}$, τCH_3
81			$\tau\text{Ph I, II}$, τCH_3
46			$\tau\text{Ph I, II}$, τCH_3
40			$\tau\text{Ph I, II}$, τCH_3
38			τCH_3

ν : stretching; δ : in-plane deformation; γ : out-of-plane deformation; ρ : rocking; τ : torsional; Ph: phenyl; I: Ph attached to methyl; II: Ph attached to fluorine; ν : very; s: strong; m: medium; w: weak; sh: shoulder; br: broad. Subscripts—a: asymmetric; s: symmetric.

The substitution of fluorine in the phenyl ring shortens the C–C bond lengths C₁₈–C₁₉ and C₁₈–C₁₇ of the benzene ring. Fluorine is highly electronegative and tries to obtain additional electron density. It attempts to draw it from the neighbouring atoms, which move closer together in order to share the remaining electrons more easily as a result. Due to this the bond angle A(17,18,19) is found to be 122.361° in the present calculation which is 120° for normal benzene. Similarly, the bond lengths C₁₈–C₁₉ and C₁₈–C₁₇ are 1.3778 and 1.3808 Å, respectively, which is 1.3864 Å for benzene. For the title compound the bond lengths C₃–O₉, C₂–N₈ are found to be 1.3594 and 1.3903 Å while for 2-mercaptobenzoxazole [29] these are, respectively, 1.3436 and 1.3739 Å. The bond lengths N₈–C₂₇, O₉–C₂₇, C₂–C₃ are found to decrease to 1.2727, 1.3470 and 1.3776 Å from the values 1.3001, 1.3804 and 1.3927 Å obtained for 2-mercaptobenzoxazole [29]. These changes in bond lengths for the title compound can be attributed to the conjugation of the phenyl ring.

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