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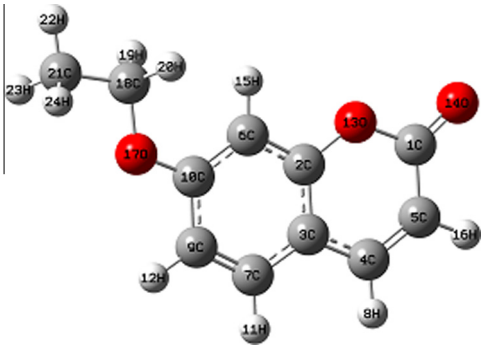
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Molecular structure and vibrational spectra of 7-Ethoxycoumarin by density functional method

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GRAPHICAL ABSTRACT



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ABSTRACT

In the present study, as a result of detailed conformational search of the 7-Ethoxycoumarin, four different conformers of (7EC) have been obtained. The FT-IR and Raman spectra of 7EC were recorded in the region 4000–400 cm^{-1} and 3500–50 cm^{-1}, respectively. Vibrational frequences of the title compound were calculated by B3LYP method using 6-311++G(d,p) basis sets. The calculated vibrational frequences were analyzed and compared with experimental results. Characteristic vibrational bands of the pyrone ring, methylene and CO groups have been identified.

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1. Introduction

Coumarins are known as benzopyrones and they have been detected in microorganisms and animal sources [1,2]. Furthermore coumarin is found a plenty of amount in a variety of plants such as tonka bean, vanilla grass, woodruff, mullein, sweet grass, lavender, sweet clover grass, and licorice, and also occurs in food plants such as strawberries, apricots, cherries, and cinnamon. And due to concerns about coumarin as a potential liver and kidney toxin, its use as a food additive is heavily restricted, although it is perfectly safe to eat foods which naturally contain coumarin [3–5].

Coumarins have inherent a variety of biological activities and have wide range of therapeutic properties. The coumarin derivatives possess different pharmacological and biological activities such as anti-inflammatory, antibacterial, vasorelaxant, antihepatitis-C virus agent, antiproliferative activity, xanthine oxidase

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inhibitor, antidiabetic, anticancer, anti-HIV, anticoagulant, spasmolytic and also used clinically for curing platelet coagulation and leucoderma [6–12]. As well as biological activities, they are commonly used as additives in food, perfumes, cosmetics, pharmaceuticals, dispersed fluorescent, electroplating adjuvant, laser dyes, insecticides and in optical brighteners. [13–15].

Additionally, the cytochrome P450 proteins are monooxygenases which catalyze many reactions involved in drug metabolism and synthesis of cholesterol, steroids and other lipids. 7-Ethoxycoumarin (7EC) is widely used as a model substrate for monooxygenase function. 7EC is metabolized by many cytochrome P450 enzymes active in foreign compound metabolism and used as a prototypic substrate to monitor P450 activity in both hepatic and extrahepatic tissues [16]. Above all, being used to determine whether isolated hepatocytes can be used to predict in vivo clearance values successfully and to develop rainbow trout liver perfusion techniques for studies on xenobiotic biotransformation, 7EC is a commonly used probe for metabolism studies [17].

However, as the best of our literature survey, there are a few experimental structural studies of coumarins [18–21]. Infrared and Raman spectroscopy is an efficient method to probe electronic and geometric structure of molecules, and has been widely used in studying the structural consequences. Moreover, vibrational spectroscopy is very important for investigation of inter- and intramolecular interactions. The *ab-initio* vibrational assignments of the infrared and Raman spectrum of molecules have been widely studied for structural investigations nowadays. In addition to this, it is known that, the different conformational structures of a compound are correlated with many of the physical and chemical properties and hence their investigation is important for drug designs and to understand several medicinal effects. Hence 7EC has shown wide variety of biological activities. It is important to determine all possible conformers and chemical activities of them.

In recent years density functional theory (DFT) methods have become a powerful tool in the investigation of molecular structures and vibrational spectra, particularly B3LYP method has been widely used [15,22–29]. The molecular geometry parameters and vibrational frequencies of some organic compounds have been calculated using B3LYP method and 6-311++G(d,p) basis set [22–24,26,29]. Similar calculations have been performed for 3-acetylcoumarin at the same level of DFT [15]. The results of these calculations brought out a close agreement between the theoretical calculations and experimental values [15,22–29].

In the present study, an exhaustive conformational search of the 7EC has been performed by combined molecular mechanic and DFT calculations. Geometry parameters and vibrational frequencies of the title compound have been calculated by B3LYP method using 6-311++G(d,p) basis sets. The calculated geometric parameters and vibrational frequencies were analyzed and compared with obtained experimental results.

2. Experimental

The 7EC powder was purchased from ABCR. FT-IR spectrum of solid 7EC was recorded in the range 4000–400 cm^{-1} on Brucker IFS 66/S with PIKE Gladi ATR (Diamond) spectrometer at room temperature with 2 cm^{-1} resolution. The FT-Raman spectrum was recorded on a Brucker FRA 106/S spectrometer using 1064 nm excitation from a Nd:YAG laser. The detector was a Gediode cooled to liquid nitrogen temperature. The upper limit for wavenumbers was 3500 cm^{-1} and the lower wavenumber is around 50 cm^{-1}. The measured FT-IR and FT-Raman spectra are shown in Figs. 1 and 2.

3. Computational details

In order to establish the stable possible conformations, the conformational space of 7EC was scanned with molecular mechanic calculations. This calculation was performed with the Spartan 08 program [30]. In the second step, geometry optimizations of all of the possible conformers was performed by B3LYP method with 6-311++G(d,p) basis set. After the most stable conformer of the title compound determined, optimized structural parameters of this conformer were used for the vibrational frequency calculations. Optimizations and frequency calculations were performed by the same level of DFT. In this step, all the calculations were performed using Gaussian 03W program package [31] with the default convergence criteria without any constraint on the geometry [32]. The assignments of the calculated wavenumbers are aided by the animation option of Gauss View 3.0 graphical interface for Gaussian programs, which gives a visual presentation of the shape of the vibrational modes along with available related molecules [33]. Furthermore, total energy distribution (TED) was calculated by using the scaled quantum mechanic program (SQM) and fundamental vibrational modes were characterized by their TED [34]. It should be noted that Gaussian 03 package does not calculate the Raman intensities. The Raman activities were transformed in to Raman intensities by using Raint program [35].

4. Results and discussion

4.1. Conformational stability and molecular structure

To found stable conformers, a meticulous conformational analysis was carried out for the title compound. Conformational space of

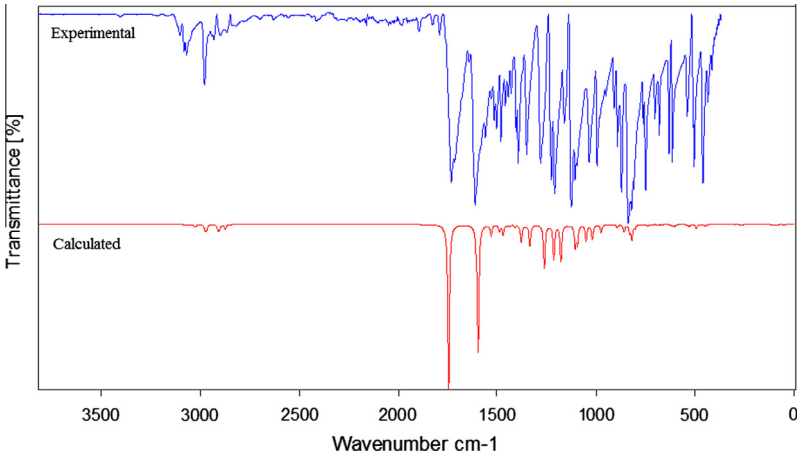


Fig. 1. Experimental and theoretical FT-IR spectra of 7EC.

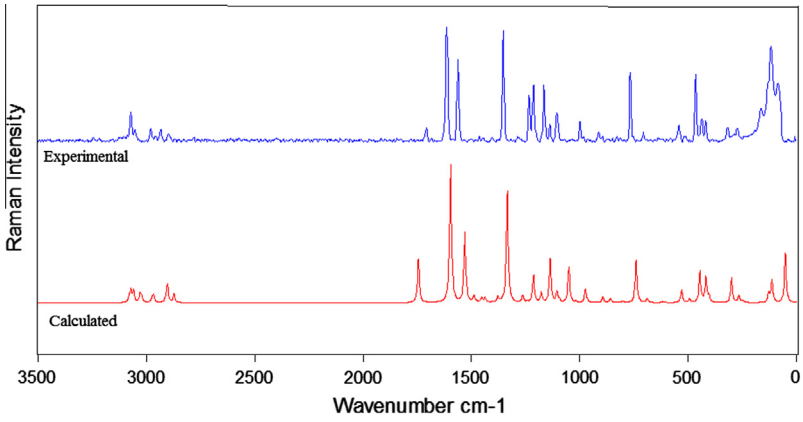


Fig. 2. Experimental and theoretical Raman spectra of 7EC.

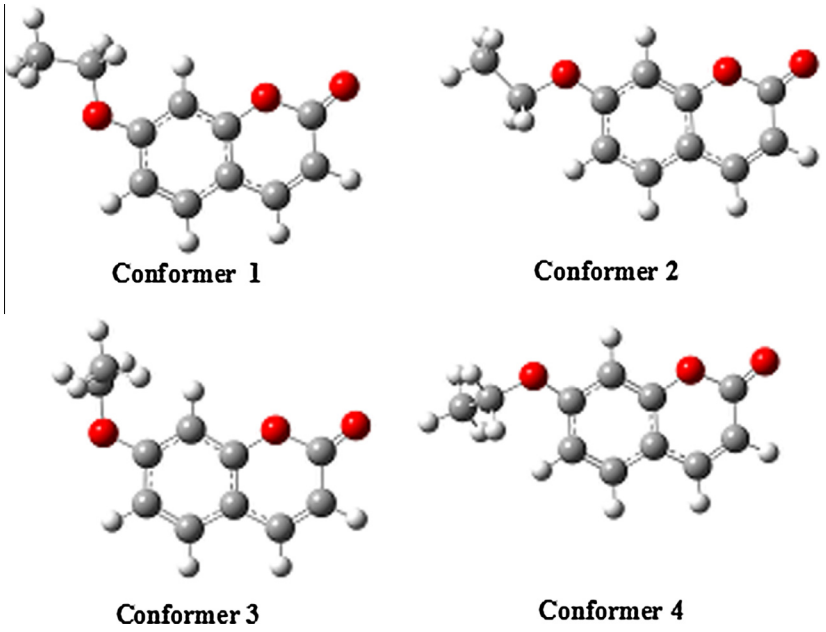


Fig. 3. Stable conformers of 7EC.

Table 1
Energetics of the conformers calculated at the B3LYP/6-311++G(d,p) level.

Conf.	E (Hartree)	E_0 (Hartree)	ΔE (kcal/mol)	Dip. mom. (D)
1	−651.046030	−650.858842	0.00	4.9107
2	−651.044643	−650.857625	0.87	7.1317
3	−651.043797	−650.856297	1.40	4.7927
4	−651.042042	−650.855072	2.50	7.2173

E_o – Zero point corrected energy.

the title compound was scanned by Molecular Mechanics Force Fields method and then full geometry optimizations of these structures were performed by B3LYP/6-311++G(d,p) method. Results of geometry optimizations were indicated that the title compound has four conformers as shown in Fig. 3. Ground state energies, zero point corrected energies (Eelect. + ZPE), relative energies and dipole moments of conformers were presented in Table 1. Zero point corrections have not caused any significant changes in the stability order. From both the calculated energies of four conformers, given in Table 1, the conformer 1 is the most stable.

The optimized geometric parameters (bond lengths, bond angles and dihedral angles) of the conformer 1 were given in Table 2 using B3LYP with 6-311++G(d,p) basis set. The atom numbering scheme adopted in this study is given in Fig. 4. In the literature, we have found neither experimental data nor calculation results on molecular structure of 7EC, therefore the molecular structure of conformer 1 of 7EC is compared with XRD data of closely related molecule tert-Butyl Coumarin-3-carboxylate [21]. A small difference between experimental and calculated geometrical parameters may come from the environment of the compound. It is clear that the experimental results belong to solid phase while theoretical calculations belong to gaseous phase. The theoretically calculated structural parameters of the all conformers of 7EC are presented in Table S1 (Supplementary information).

Because the conformer 1 is the most stable one, and the calculated wavenumbers of conformer 1 also show good correlation with the experimental FT-IR and Raman spectra, as it will be seen in the Table 3, from this point the discussion will be based on conformer 1, further in this paper.

4.2. Vibrational assignments

The 7EC molecule has 24 atoms, which possess 66 normal modes of vibrations. All the vibrations are active in the infrared

Table 2
The calculated geometric parameters of 7EC by B3LYP/6-311++G(d,p) method, bond lengths in angstrom (Å) and angles in degrees(°).

Parameters	Calculated	Experimental[a]		Calculated	Experimental[a]
Bond lengths (Å)			*Bond angles*		
C_1—C_5	1.45	1.463	C_6—C_{10}—O_{17}	124.2	–
C_1—O_{13}	1.40	1.383	C_9—C_{10}—O_{17}	115.5	–
C_1—O_{14}	1.20	1.202	C_1—O_{13}—C_2	123.0	122.8
C_2—C_3	1.40	1.389	C_{10}—O_{17}—C_{18}	119.4	–
C_2—C_6	1.39	1.372	O_{17}—C_{18}—C_{21}	107.6	–
C_2—O_{13}	1.36	1.369	*Selected dihedral angles*		
C_3—C_4	1.43	1.437	O_{13}—C_1—C_5—C_4	0.0	5.94
C_3—C_7	1.41	1.390	O_{14}—C_1—C_5—C_4	180.0	173.1
C_4—C_5	1.35	1.344	C_5—C_1—O_{13}—C_2	0.0	3.1
C_6—C_{10}	1.39	1.359	O_{14}—C_1—O_{13}—C_2	180.0	176.0
C_7—C_9	1.38	1.370	C_6—C_2—C_3—C_4	180.0	–
C_9—C_{10}	1.41	1.375	C_6—C_2—C_3—C_7	0.0	–
C_{10}—O_{17}	1.35	–	O_{13}—C_2—C_3—C_4	0.0	2.49
O_{17}—C_{18}	1.44	–	O_{13}—C_2—C_3—C_7	180.0	–
C_{18}—C_{21}	1.52	–	C_3—C_2—C_6—C_{10}	0.0	–
Bond angles			O_{13}—C_2—C_6—C_{10}	180.0	179.4
C_5—C_1—O_{13}	115.8	117.6	C_3—C_2—O_{13}—C_1	0.0	1.0
C_5—C_1—O_{14}	126.8	127.0	C_6—C_2—O_{13}—C_1	180.0	–
O_{13}—C_1—O_{14}	117.4	116.9	C_2—C_3—C_4—C_5	0.0	0.36
C_3—C_2—C_6	122.0	122.9	C_7—C_3—C_4—C_5	180.0	176.1
C_3—C_2—O_{13}	121.2	120.7	C_2—C_3—C_7—C_9	0.0	0.5
C_6—C_2—O_{13}	116.8	117.4	C_4—C_3—C_7—C_9	180.0	–
C_2—C_3—C_4	117.5	117.4	C_3—C_4—C_5—C_1	0.0	4.6
C_2—C_3—C_7	117.8	–	C_2—C_6—C_{10}—C_9	0.0	–
C_4—C_3—C_7	124.7	124.1	C_2—C_6—C_{10}—O_{17}	180.0	–
C_3—C_4—C_5	121.0	120.8	C_3—C_7—C_9—C_{10}	0.0	–
C_1—C_5—C_4	121.5	121.3	C_7—C_9—C_{10}—C_6	0.0	–
C_2—C_6—C_{10}	118.8	–	C_7—C_9—C_{10}—O_{17}	180.0	–
C_3—C_7—C_9	121.2	–	C_6—C_{10}—O_{17}—C_{18}	0.0	–
C_7—C_9—C_{10}	119.9	–	C_9—C_{10}—O_{17}—C_{18}	180.0	–
C6—C10—C9	120.3	–	C_{10}—O_{17}—C_{18}—C_{21}	180.0	–

[a] Values are taken from Ref. [21].

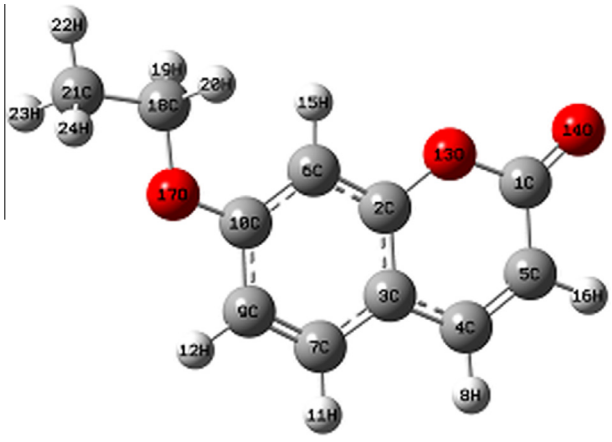


Fig. 4. Atom numbering scheme adopted in this study.

and Raman spectra. Usually the calculated harmonic vibrational wavenumbers are higher than the experimental ones, because of the anharmonicity of the incomplete treatment of electron correlation and of the use of finite one-particle basis set. The harmonic frequencies were calculated by B3LYP method using 6-311++G(d,p) basis set and then scaled by 0.967 (for wavenumbers fewer than 1800 cm^{-1}) and 0.955 (for those more than 1800 cm^{-1}) [22–24].

Experimentally observed and theoretically calculated harmonic vibrational frequencies and their correlations were gathered in Table 3. From the calculations, the computed values are in good agreement with the observed values. The vibrational bands assignments have been made by using the animation option of Gauss View 3.0 graphical interface for Gaussian programs [36] along with available related molecules and also by means of TEDs using the SQM program [37].

4.2.1. CH vibrations

The aromatic CH stretching vibrations of heteroaromatic structure are expected to appear in the 3100–3000 cm^{-1} frequency ranges, with multiple weak bands. The nature of substituents can not affect much to the bands in this region [38,39]. The CH in-plane bending vibrations appear by sharp but weak to medium intensity bands in the 1100–1500 cm^{-1} region. These bands are not sensitive to the nature of substituents [40]. The out-of-plane bending vibrations occur in the wavenumber range 800–1000 cm^{-1} [39].

The aromatic C—H stretching vibrations of the title compound were observed at 3082, 3069, 3029 and 3011 cm^{-1} in FT-IR spectrum and at 3096, 3072 and 3053 cm^{-1} in FT-Raman spectrum. All predicted wavenumbers of CH stretching vibrations are in the 3100–3000 cm^{-1} frequency ranges (mode nos.: 1,2,3,4,5) and well reproduced the experimental ones in the infrared and Raman spectrum.

The in-plane CH bending vibrations of rings were observed at 1501,1428, 1257, 1225, 1208, 1160, 1106, 1094 and 980 cm^{-1} in FT-IR spectrum and the bands at 1233, 1213, 1176, 1105 cm^{-1} in FT-Raman spectrum (mode nos.: 15, 19, 25, 26, 27, 28,30,31, 32,35). The band observed at 951,910, 838 and 781 cm^{-1} in the infrared spectrum (mode nos.: 36, 37, 40, 41, 44) and the band observed at 910 cm^{-1} in the Raman spectrum were assigned to out-of-plane CH vibrations. The calculated wave numbers of in-plane and out-of-plane CH bands well reproduced the experimental ones in the infrared and Raman spectrum.

For the assignments of CH_3 group frequencies, eight fundamental vibrations can be associated to CH_3 groups. Three stretching,

Table 3
Comparision of the observed and calculated vibrational spectra of 7EC.

Mode nos.	Experimental wavenumbers (cm^{-1})		Theoretical wavenumbers (cm^{-1}) B3LYP				TED[c](%)
	IR	Raman	Unscaled[a]	Scaled[b]	I_{IR}	I_{Raman}	
1	3082	3096	3225	3080	0	3	99ν(CH), ring
2	–	3072	3216	3072	0	9	97ν_s(CH), pyr
3	3069	3053	3203	3059	0	8	93ν_s(CH), ring
4	3029	–	3172	3029	1	6	91ν_{as}(CH), ring
5	3011	–	3164	3021	1	4	94ν_{as}(CH), pyr
6	2978	2980	3115	2975	4	3	96ν_{as}(CH_3)
7	2960	2960	3107	2967	3	5	98ν_{as}(CH_3)
8	2931	2933	3048	2910	3	3	96ν_{as}(CH_2)
9	2898	2889	3040	2903	3	13	98ν_s(CH_3)
10	2867	–	3008	2873	3	6	99ν_s(CH_2)
11	1732	1706	1803	1743	100	33	24ν(C=O) + 21ν(CC) + 15δCCH + 14δCCO
12	–	–	1657	1602	5	7	31ν(C=C) + 30δCCH + 17δCCC
13	1608	1612	1649	1594	75	100	30ν(C=C) + 30δCCH + 15δCCC
14	1558	1561	1581	1529	6	52	35ν(C=C) + 21δCCH + 15δCCC + 14δCCO
15	1501	–	1538	1487	4	5	31δ(CH), ring + 18 δ(CH_2), sciss + 16ν(C=C)
16	1480	–	1519	1468	6	0	29δ(CH_2), sciss + 18 δ_d(CH_3)+17δ(CH)
17	1458	–	1501	1452	1	3	42δ_d(CH_3) + 29(CH_2), sciss
18	1442	–	1486	1436	1	3	68δ_d(CH_3)
19	1428	–	1457	1409	1	0	43δ(CH), ring + 20ν(C=C) + 10δ(CCC)
20	1402	–	1432	1385	1	0	35δ_d(CH_3) + 11νCC + 10δHCH
21	1392	–	1424	1377	10	4	43δ_s(CH_3), umbrella + 11νCC + 11δHCH
22	–	–	1402	1356	1	1	54δ(CH_2), waging + 16δHCH + 10δOCH
23	1350	1352	1379	1333	13	83	36ν(C=C)+15δCCH + 12δCCC
24	1280	1286	1306	1263	0	3	53δ(CH_2), twist + 16δOCH + 10γCOCH
25	1257	–	1304	1261	26	2	31δ(CH), ring + 15ν(C=C) + 12δCCC + 11νOC
26	1225	1233	1285	1242	0	1	48δ(CH), ring + 14δCCC + 13ν(C=C)
27	1208	1213	1254	1213	21	20	42δ(CH), ring + 24ν(C=C) + 11δCCC
28	1160	1176	1217	1177	22	7	40δ(CH), ring + 14νOC + 10ν(C=C) + 10δCCC
29	1125	1137	1177	1138	0	0	53 δ(CH_2), rocking t + 12δOCH + 11γOCCH + 10γCOCH
30	–	–	1175	1136	0	32	58δ(CH), ring + 14ν(C=C) + 10νOC
31	1106	1105	1143	1105	13	8	36δ(CH), ring + 10νCC + 10γHCCH
32	1094	–	1131	1094	11	2	34δ(CH), ring + 17γHCCH
33	1034	–	1086	1050	10	26	29δCCH + 20νCC + 15νOC + 13δCCC
34	995	999	1054	1019	9	1	24δCCH + 23νCC + 18νOC
35	980	–	1007	974	5	9	28δ(CH), ring + 22νCC + 17δCCC + 10νOC
36	951	–	999	966	0	1	64γ(CH), ring + 13 γ(OH)
37	910	910	961	929	0	0	66γ(CH), ring + 13 γ(OH) + 12γ(CC)
38	893	896	924	894	2	4	23δ(CH_3), rocking + 16γHCCH + 13δCCC
39	871	–	888	859	4	3	25δCCC + 20δCCH + 13ν(C=C) + 12δCCO + 11νOC
40	–	–	858	830	4	0	47γ(CH), ring + 14γCCCC
41	838	–	847	819	9	0	42γ(CH), ring + 22 γ(OH) + 11γ(CC)
42	810	–	831	804	1	0	20τOCCH + 19τHCCH + 15δCCH + 14γHCCC + 12γCCCC
43	–	–	829	801	1	1	18δCCH + 15δCCC + 14νOC + 13ν_{as}(C=C)+12δCCO
44	781	–	815	788	0	0	47γ(CH), ring + 21γ(OH)
45	762	767	765	740	1	32	47δCCC + 14δCCH + 10δOCC + 10νOC
46	703	707	746	721	0	0	33τCCCC + 29τHCCC + 13τCCOC + 10τOCCH + 10τOCCC
47	682	–	712	689	0	3	22δCCC + 17δCCH + 14δOCC + 12ν(CC)
48	667	–	688	665	0	0	32τHCCC + 31γCCCC + 10γCCOC + 10γOCCH
49	616	–	640	619	1	1	25τHCCC + 21τCCCC + 16γCCCO + 15τCCOC + 10τOCCH
50	–	–	626	605	1	0	35δCCC + 24δCCH + 14δOCC + 10ν(CC)
51	540	543	548	530	1	10	23δCOC + 20δCCH + 20δOCC + 10ν(CC)
52	505	–	511	494	2	3	19δOCC + 18δCCC + 12δCCH
53	461	466	467	451	1	0	38γCCCC + 29τHCCC + 12γCCOC
54	436	437	461	446	0	23	27δOCC + 23δCCC + 16δCCH + 11νCC + 11δCOC
55	417	420	433	418	0	19	21δOCC + 20δCCC + 19δCCH
56	407	–	418	404	0	4	32γCCCC + 19γHCCC + 18τCCCO + 11τCCOC + 10τHCCO
57	–	318	311	300	0	18	22δCCC + 17δCCH + 11νCC
58	–	273	276	267	0	5	22δOCC + 15δCCC + 14δCCH
59	–	–	275	266	1	1	39τ(CH_3) + 16τCCCC + 14τCCCO + 12τCCOC + 10τHCCC
60	–	–	258	249	0	2	24γCCCO + 22γCCCC + 20γCCOC + 12γHCCC
61	–	–	250	242	0	0	47τ(CH_3) + 27τOCCH
62	–	–	133	129	0	7	Lattice mode
63	–	118	118	114	0	17	Lattice mode
64	–	–	110	106	0	0	Lattice mode
65	–	86	89	86	1	0	Lattice mode
66	–	–	54	53	0	37	Lattice mode

υ, stretching; δ, in-plane bending; γ, out-of-plane bending; τ, torsion.
Relative absorption intensities and Raman intensities normalized with highest peak absorption equal to 100.
[a] Unscaled calculated wavenumbers.
[b] Obtained from the wave numbers calculated at B3LYP/6-311++G(d,p) using scaling factors 0.967 (for wave numbers under 1800 cm^{-1}) and 0.955 (for those over 1800 cm^{-1}.
[c] Total energy distribution calculated B3LYP/6-311++G(d,p) level of theory. Only contributions $\geqslant$10% are listed.

one umbrella, one rocking and three deformation vibration mode designated the motion of the methyl group [41,42]. For the methyl group vibrations, the bands observed at 2978, 2960 cm^{-1} in FT-IR spectrum and the bands observed at 2980 and 2960 cm^{-1} in Raman spectrum were assigned to CH_3 antisymmetric stretching vibrations (mode nos. 6, 7). The CH_3 symmetric stretching vibrations were observed at 2898 cm^{-1} in the FT-IR spectrum. In the Raman spectrum, these vibration was observed at 2889 cm^{-1} (mode no. 9).The theoretically predicted asymmetric and symmetric CH_3 stretching vibrations show good agreement with the experimental values. The bands observed at 1458, 1442 and 1402 cm^{-1} in the FT-IR spectrum were assigned to deformation bending (mode nos. 17, 18, 20); the band observed at 1392 cm in the FT-IR spectrum was assigned to symmetric bending (mode no. 21); the band observed at 893 cm^{-1} in the FT-IR and the band observed at 896 cm^{-1} in the Raman spectrum were assigned to rocking vibrations of CH3 (mode no. 38). The experimental and theoretical wavenumbers of CH_3 group vibrations show the good correlation with the literature data [25–27].

The antisymmetric stretching ($\nu_{as}CH_2$) and symmetrical stretching (ν_sCH_2) bands of methylene groups occur at 2931 and 2867 cm^{-1} in the FT-IR spectrum, respectively (mode nos. 8, 10). In addition, the band observed at 2933 cm^{-1} in the Raman spectrum was decided the antisymmetric stretching ($\nu_{as}CH_2$) of methylene groups. The four bending vibrations of C—H bonds in the methylene groups are referred to as scissoring, twisting, wagging and rocking and they are identified. The scissoring mode is characterized by the IR band at 1480 cm^{-1} which is computed at 1468 cm^{-1}. In 7EC the wagging vibrations of CH_2 are found in both IR and Raman spectrum near 1350 cm^{-1} which is justified by our DFT calculation also. The twisting and rocking vibrations of CH_2 group are observed at 1280 cm^{-1} and 1125 cm^{-1} in FT-IR spectrum respectively which is observed at 1286 cm^{-1} and 1137 cm^{-1} in Raman spectrum.

4.2.2. CO vibrations

Two different type CO stretching vibrations are observed at coumarine derivatives. The first one is C=O and the second one is C—O streching vibrations. The C=O stretching vibrations are found in the region 1780–1700 cm^{-1} [28,29]. The C_1—O_{13} and C_2—O_{13} vibrations of pyrone rings of other coumarins were observed in the 1250–850 cm^{-1} region [28,29]. In this study, the band appeared at 1732 cm^{-1} (FT-IR) and 1706 cm^{-1} (FT-Raman) are belongs to C=O group, but according to the TED, as it is seen in Table 3, these are not pure modes. The corresponding calculated wavenumber is at 1743 cm^{-1} (mode no.: 11) using B3LYP/ 6-311++G(d,p) basis set. In this study, the C_1—O_{13} and C_2—O_{13} stretching vibrations were observed at 1257 and 1034 cm^{-1} in FT-IR spectrum (mode nos.: 25, 33). In addition to this, the bands observed at 1160, 995 cm^{-1} and the Raman conterparts of them observed at 1176, 999 cm^{-1} include C_{10}—O_{17} and C_{18}—O_{17} stretching vibrations (mode nos.: 28, 34) but according to the TED, as it is seen in Table 3, these are not pure modes.

4.2.3. CC vibrations

The compound 7EC consists of hetero aromatic ring fused with aromatic benzene ring system. The aromatic ring carbon–carbon stretching modes appear in the region of 1650–1200 cm^{-1} [15]. Therefore, the vibrational frequency at 1608, 1558, 1350 in FT-IR spectrum and at 1612, 1561 and 1352 in Raman spectrum (mode no.: 12, 13, 14 and 23) were assigned to C—C stretching vibrations respectively.

4.2.4. Some low-frequency vibrations

Certain Raman bands observed below 150 up to 100 cm^{-1} and still low-frequency bands have to be interpreted as arising from the lattice vibrations. In this work, Raman bands in the 54–133 cm^{-1} spectral range are simply defined as lattice vibrations. In the title compound, there are two Raman bands at 118 and 86 cm^{-1}. In this region, the predicted bands are: 133 cm^{-1}, 118 cm^{-1}, 110 cm^{-1}, 89 cm^{-1} and 54 cm^{-1} by using the B3LYP/6-311++G(d,p) level of theory.

5. Conclusion

The FT-IR and FT-Raman spectra of 7EC were studied. The equilibrium geometries, harmonic wavenumbers, ground state energy, and dipole moment were calculated for the first time. The calculated vibrational values are in good agreement when they are compared with IR and Raman experimental data. Gaussian 03 and Spartan programs were used to find the most stable conformer of 7EC.

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Appendix A. Supplementary material

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.molstruc.2013.06.026.

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