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Molecular geometry and vibrational analysis of 1-(2, 5-dimethyl-furan-3-yl)-ethanone by using density functional theory calculations

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ABSTRACT

In this work, we obtained the vibrational spectra of 1-(2,5-dimethyl-furan-3-yl)-ethanone (1DF3E) by using Density functional theory (DFT) calculations. Normal coordinate analysis also carried out to the titled compound in order to support the vibrational spectra of (1DF3E). After that, the results obtained from these calculations are compared with the Experimental (FT-IR, FT-Raman) values. By using the scaling procedure, the observed wave numbers from FT-IR and FT-Raman are analyzed with the help of theoretically obtained vibrational spectra. The assignments of bands to various normal modes of the molecules were also carried out.

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1. Introduction

Furan is 5-membered heterocyclic oxygen containing unsaturated ring compound. Furan shows aromatic properties because the resulting π molecular orbital satisfies the Huckel's rule (n = 1 in 4n + 2). The Furan nucleus is also found in a large number of biologically active materials. Furan ring is an important constituent in syn fuel products that are of major interest in the coal conversion industry. Furan ring as an important group of heteroaromatic compounds that have been found in many natural products and substances that have useful in industrial applications [1]. It is often used as synthetic intermediates in the preparation of acyclic, carbocyclic and heterocyclic compounds and its derivatives as well as some other heterocyclic compounds are of great interest due to their application of molecules to characterize the active sites in Zeolites. Many researchers show their special interest to study the compound 2-furoic acid because of its extraordinary pharmaceutical and industrial importance. They exhibit anti-inflammatory, anti-irritant and anti-microbial effects, which make them more potent for topical applications in cosmetic and pharmaceutical formulations.

In addition, furan carboxylic acids find applications in the agrochemical field as compounds which enhance plant resistance to stress and in polymer chemistry for nylon preparation. Further, it possesses high optic non-linearity which can be used in the fabrication of optical and electroluminescent devices [2].

Vibrational spectroscopy is one of the most widely used methods in spectroscopy and it has been proven to be a powerful technique in the determination of the structural properties of various biologically active compounds. The theoretical and experimental studies on vibrational spectra of furan and its derivatives have been reported in literature time to time. El-Azhary et al studied the vibrational spectrum of Furan and Thiophene at B3LYP, MP2 and HF method of theory which shows good coincidence between the experimental and theoretical results [3]. Lucy W. Pickett studied the vibrational analysis of the absorption spectrum of Furan in the Schumann Region [4]. -Bharanidharan et al studied the Vibrational Spectral Analysis and First Order Hyperpolarizability Calculations on (E)-N′-(furan-2-yl methylene) Nicotinohydrazide [5] and found that calculated values are good agreement with the experimental values.

However, literature survey indicates that there is no detailed study of quantum chemical calculations for the title compound. Hence, in the present study, we report quantum chemical calculations by using experimental (FT-IR and FT-Raman) and Density

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functional calculations of 1-(2,5-dimethyl-furan-3-yl)-ethanone for the first time.

2. Materials and methods

The studied compound 1-(2,5-dimethyl-furan-3-yl)-ethanone [CAS 10599-70-9] whose structure formula are shown in Fig. 1, were obtained commercially from Aldrich Chemical Co., with assessed purity of greater than 98% respectively and used in subsequent spectroscopic investigations without any further purification.

2.1. FT-IR spectrum

FT-IR spectrum o of the investigated compound was recorded at 302.50° Kelvin temperature in the range 4000–400 cm^{-1} using Nicolet 6700 FTIR spectrometer furnished with a Thermo Nicolet Continuum IR microscope and by a Renishaw in via Raman microscope with UV or visible laser excitation at a resolution of ±4 cm^{-1}.

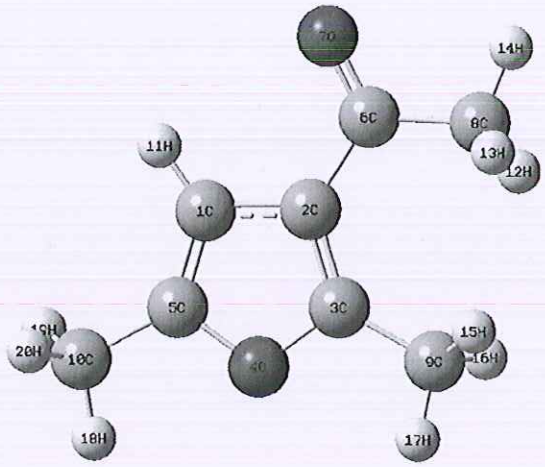

Fig. 1. Molecular structure of 1-(2,5-dimethyl-furan-3-yl)-ethanone along with numbering of atom.

2.2. FT-Raman spectrum

The FT-Raman spectrum of the compound (1DF3E) was measured at a 2 cm^{-1} resolution with a Nicolet Magna 750 Raman spectrometer instrumented with an InGaAs sample detector. The excitation source utilized was the 1064-nm line from Neodymium: Yttrium Aluminium Garnet laser. The laser power at the sample location was typically 450 mW.

2.3. Computational details

All the quantum chemical calculations in this work was performed using Gaussian 09 software program package [6] at theBecke-3-Lee-Yang-Parr (B3LYP) level augment with DFT/B3LYP/6-311++G** basis set. Transformation of force field, subsequent normal coordinate analysis including least square refinement of the scaling factors, total energy distribution (TED) and IR, Raman intensities were done on a PC with MOLVIB program (version 7.0 G77) written by Sundius [7,8]. The Raman activity (Si) calculated by Gaussian 09 and adjusted during scaling procedure with MOLVIB are converted to relative Raman intensity (I_i) using the following relation from the basic theory of Raman scattering

$$I_i = \frac{f(\upsilon_o - \upsilon_i)^4 Si}{\upsilon_i\left(1 - \exp\left(\frac{-hc\upsilon i}{kT}\right)\right)}$$

here ν_o is the exciting frequency (in cm^{-1} units), ν_i is the vibrational wave number of the normal mode, h, c and K are the universal constants and f is suitably chosen common normalization factor for all the intensities.

Table 1
Optimized geometrical parameters of 1-(2,5-dimethyl-furan-3-yl)-ethanone obtained by B3LYP/6-31G(d,p) and B3LYP/6-311++G** density functional calculations.

Bond length (Å)[a]			Exp.	Bond angle (Å)[a]			Exp.
B3LYP/6-31G(d,p)		B3LYP/6-311++G(d,p)		B3LYP/6-31G(d,p)		B3LYP/6-311++G(d,p)	
C1-C2	1.441	1.443	1.429	C1-C2-C3	106.09	106.15	106.26
C2-C3	1.378	1.376	1.362	C2-C3-O4	109.27	109.15	109.39
C3-O4	1.362	1.361	1.363	C3-O4-C5	108.31	108.44	107.44
O4-C5	1.380	1.380	1.379	O4-C5-C1	109.17	109.10	109.44
C5-C1	1.355	1.352	1.335	C5-C1-C2	107.14	107.14	107.47
C2-C6	1.475	1.475	1.473	C1-C2-C6	123.26	123.47	128.51
C6-O7	1.224	1.220	1.231	C3-C2-C6	130.36	130.36	125.23
C6-C8	1.520	1.517	1.469	C2-C3-C9	135.74	135.78	134.68
C3-C9	1.493	1.491	1.474	O4-C3-C9	114.97	115.06	115.93
C5-C10	1.488	1.485	1.488	O4-C5-C10	116.33	116.40	–
C1-H11	1.080	1.077	–	C1-C5-C10	134.48	139.47	134.70
C8-H12	1.096	1.093	–	C2-C6-O7	120.10	120.11	120.82
C8-H13	1.096	1.094	–	C2-C6-C8	118.08	118.11	117.73
C8-H14	1.091	1.088	–	C8-C6-O7	120.47	120.41	121.44
C9-H15	1.095	1.092	–	C5-C1-H11	127.63	127.43	–
C9-H16	1.096	1.093	–	C2-C1-H11	125.22	125.42	–
C9-H17	1.093	1.090	–	C6-C8-H12	111.32	111.09	–
C10-H18	1.097	1.094	–	C6-C8-H13	111.01	110.84	–
C10-H19	1.093	1.090	–	C6-C8-H14	108.65	108.72	–
C10-H20	1.097	1.094	-	C3-C9-H15	111.97	111.81	–
				C3-C9-H16	112.01	111.80	–
				C3-C9-H17	109.13	109.10	–
				C5-C10-H18	111.58	111.39	–
				C5-C10-H19	109.68	109.65	–
				C5-C10-H20	111.58	111.33	–

[a] For numbering of atoms refer Fig. 1.

3. Results and discussion

3.1. Molecular geometry

The labeling and symbol of the investigated compound was shown in (Fig. 1). The most optimized structural parameters i.e. bond length and a bond angle at two different basis sets was reported in (Table 1). The global minimum energies obtained from two different basis sets were tabulated in (Table 2). From the (Table 2), the energy difference is clearly comprehensible, since the molecules are under different environments. The examined compound belongs to C_1 point group symmetry with 20 atoms forms the structure. The molecule has 54 fundamental modes of vibration. From the structural point of view of the molecule 1DF3E have

$$\Gamma_{vib} = 37A'(\text{in - plane}) + 17A''(\text{out - of - plane})\text{vibrations}$$

3.2. Vibrational analysis

Complete illustration of vibrational modes can be given by means of normal coordinate analysis (NCA). For this reason, the specified 54 standard internal coordinates are refined and tabulated in (Supplementary Data 1). From these a non-redundant set of local symmetry coordinates were constructed by suitable linear combination of internal coordinates following the recommendations of Fogarasi et al. [9,10] are presented in (Table 3). The Simulated and Experimental FT-IR and FT-Raman spectrums were shown in Figs. 2 and 3. Comparison between the calculated and observed vibrational spectra helps us to understand the observed spectral features. The results of our vibrational analysis, viz., calculated un-scaled vibrational frequencies and IR intensities, SQM frequencies, potential energy distributions (PED) and assignment of the fundamentals, for the title compound are collected in (Table 4). Frequencies, refinement of scaling factors were applied and optimized via least square refinement algorithm which resulted a weighted RMS deviation of 3.1 cm^{-1} between the experimental and scaled quantum mechanical (SQM) frequencies for 6-311++G** basis set.

Table 2
Total energies (in Hartrees) based on B3LYP/6-31G** and B3LYP/6-311++G** basis sets for 1-(2,5-dimethyl-furan-3-yl)-ethanone.

Basis Set	1-(2,5-Dimethyl-furan-3-yl)-ethanone
B3LYP/6-31G(d,p)	−461.31437342
B3LYP/6-311++G(d,p)	−461.44449187

3.2.1. CH vibrations

The CH stretching Vibration mode was observed at 3114 cm^{-1} in FT-IR and 3113 cm^{-1} in FT-Raman Spectrum which was good coincidence with theoretically calculated wave number at 3113 cm^{-1}.

3.2.2. C—C vibrations

Many ring modes are affected by the substitutions in the ring of 1DF3E. In the present study the bands identified at 501, 531, 391 and 174 cm^{-1} for 1DF3E have been designated to ring in-plane and out-of-plane bending modes, respectively by careful consideration of their quantitative descriptions. A small change in frequencies observed for these modes are mainly due to the presence of methyl group in 1DF3E and from different extents of mixing between ring and constituent group vibrations.

Table 3
Definition of local-symmetry coordinates and the values of corresponding scale factors used to correct the B3LYP/6-311++G** force field calculations of 1-(2,5-dimethyl-furan-3-yl)-ethanone.

No. (i)	Symbol[a]	Definition	Scale factors
Stretching			
1–3	ν(C—C)	R1, R2, R3	0.941
4–7	ν(C—C)(Sub)	R4, R5, R6, R7	1.049
8	ν(C—H)ar	R8	0.910
9–11	νCH3ss	(R9 + R10 + R11)/√2, (R12 + R13 + R14)/√2, (R15 + R16 + R17)/√2	0.915
12–14	νCH3ips	(2R9 − R10 − R11)/√6, (2R12 − R13 − R14)/√6, (2R15 − R16 − R17)/√6	0.915
15–17	νCH3ops	(R10 − R11)/√2, (R13 − R14)/√2, (R16 − R17)/√2	0.915
18–19	ν(C-O)	R18, R19	0.908
20	ν(C-O)sub	R20	0.942
In-plane Bending			
21	βRsym	β21 + a(β22 + β25) + b(β23 − β24)	1.102
22	βRasy	(a − b)(β22 − β25)+(1 − a)(β23 + β24)	1.102
23–25	βCH3sb	(−γ26 − γ27 − γ28 + γ35 + γ36 + γ37)/√6,(−γ29 − γ30 − γ31 + γ38 + γ39 + γ40)/√6, (−γ32 − γ33 − γ34 + γ41 + γ42 + γ43)/√6	0.998
26–28	βCH3ipb	(−γ35 − γ36 − 2γ37)/√6, (−γ38 − γ39 − 2γ40)/√6, (−γ41 − γ42 − 2γ43)/√6	0.998
29–31	βCH3opb	(γ35 − γ36)/√2, (γ38 − γ39)/√2, (γ41 − γ42)/√2	0.998
32–34	βCH3ipr	(2γ26 − γ27 − γ28)/√6, (2γ29 − γ30 − γ31)/√6, (2γ32 − γ33 − γ34)/√6	0.998
35–37	βCH3opr	(γ27 − γ28)/√2, (γ30 − γ31)/√2, (γ33 − γ34)/√2	0.998
38	βCH	(γ44 − γ45)/√2	1.044
39	βCO sub	(γ46 − γ47)/√2	0.937
40–42	βCC	(γ48 − γ49)/√2, (γ50 − γ51)/√2, (γ52 − γ53)/√2	0.937
43	βCC sub	(γ54 − γ55)/√2	0.844
Out of plane bending			
44	ωC—H	ρ 56	0.874
45	ωC—O	ρ 57	0.986
46–48	ωC—C	ρ 58, ρ 59, ρ 60,	0.986
Torsions			
49	R2torsion1	τ63 + b(τ61 + τ65) + a(τ62 + τ64)	0.983
50	R2torsion2	(a − b)(τ64 − τ62) + (1 − a)(τ63 − τ61)	0.983
51–53	τC—CH3	(τ66 + τ67 + τ68)/2, (τ69 + τ70 + τ71)/2, (τ72 + τ73 + τ74)/2	0.866
54	τCCCC	(τ75 + τ76)/2	0.981

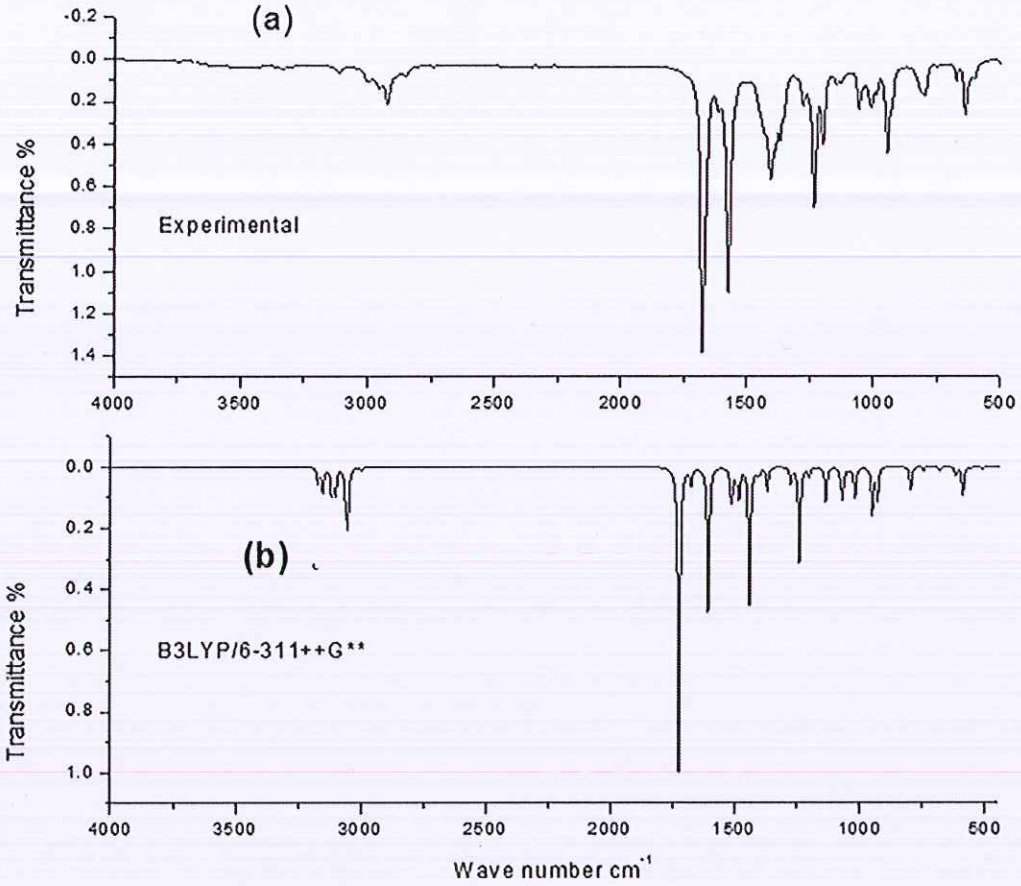

Fig. 2. (a) Experimental, (b) Simulated FT-IR spectra of 1-(2, 5-dimethyl-furan-3-yl)-ethanone.

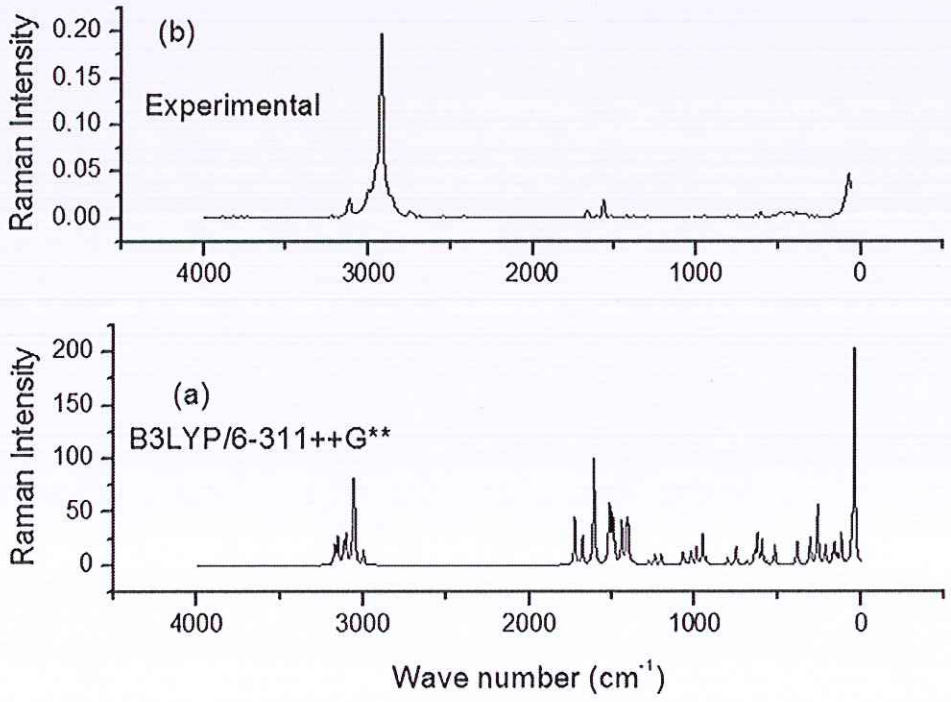

Fig. 3. (a) Simulated FT-Raman spectra of 1-(2, 5-dimethyl-furan-3-yl)-ethanone (b) Experimental FT-Raman spectra of 1-(2, 5-dimethyl-furan-3-yl)-ethanone.

Table 4
Detailed assignments of fundamental vibrations of 3-Acetyl-2,5-dimethylfuran normal mode analysis based on SQM force field calculations using B3LYP/6-311++G**.

S. No.	Symmetry species	Experimental (cm^{-1})		Scaled frequencies (cm^{-1})	Un-scaled frequencies (cm^{-1})	Intensity		Characterization of normal modes[a] with PED (%)[d]
		FT-IR	FT-Raman			I_{IR}[b]	I_{RA}[c]	
1	A′	3113	3114	3113	3261	8.7146	4.750648	νCHar (98)
2	A′	3007	3003	3008	3140	11.502	0.41401	νCH3op (71), νCH3ip (24)
3	A′	2992		2993	3123	1.852	13.16679	νCH3op (79), νCH3ip (14)
4	A′	2988		2989	3120	0.6038	0.292813	νCH3ip (92), νCH3ss (5)
5	A′	2962		2962	3091	0.087	0.088426	νCH3ip (67), νCH3op (25)
6	A′	2957	2957	2957	3085	1.8064	0.70246	νCH3ip (68), νCH3op (16)
7	A″	2942	2930	2942	3072	4.9906	4.905393	νCH3op (98)
8	A″	2905	2904	2905	3034	8.001	0.454354	νCH3ss (93)
9	A‟	2903		2903	3032	12.392	9.453981	νCH3ss (89)
10	A″	2895	2860	2895	3025	100	0.300667	νCH3ss (88)
11	A′	1676	1666	1676	1724	28.427	0.540928	νCOsub (9)
12	A′	1626	1608	1632	1655	0.4438	1.292159	νCC (50), βRasy (16), νCCsub (12)
13	A′	1571	1565	1569	1587	2.9964	8.140201	νCC (46), νCCsub (15), βCH3ib (13)
14	A′	1494	1511	1491	1493	3.2212	0.060308	βCH3ib (42), βCH3ob (41)
15	A′	1489		1486	1489	32.9688	1.208872	βCH3ib (52), βCH3ob (42)
16	A″	1488		1484	1487	10.3392	0.142916	βCH3ob (86)
17	A′	1474		1471	1473	1.1626	5.58439	βCH3ob (56), βCH3ib (41)
18	A′	1473		1470	1473	5.7128	0.278754	βCH3ob (89)
19	A′	1465		1462	1464	2.8964	0.183638	βCH3ob (49), βCH3ib (42)
20	A′	1431		1427	1431	6.7182	4.750648	βCH3ib (48), βCH3sb (41)
21	A′	1420	1422	1416	1419	6.1084	0.41401	βCH3sb (50), βCH3ib (49)
22	A′	1402		1406	1411	27.294	13.16679	βCH3sb (51), βCH3ib (48)
23	A′	1368		1377	1380	0.3658	0.292813	βCH3ib (52), βCH3sb (47)
24	A′	1277	1301	1288	1282	48.127	0.088426	βRsym (40),νCO (10)
25	A″	1232	1221	1237	1245	0.9648	0.70246	βCH3sb (20), νCO (20), βCH3ib (14)
26	A′	1198	1189	1195	1202	11.331	4.905393	βCH3ib (21), βCH (19), βCH3sb (17), νCCsub (16)
27	A′	1145	1146	1145	1152	0.138	0.454354	νCC (25), βCH3ib (13), βCH (12)
28	A′	1128	1086	1084	1074	1.884	9.453981	βRasy (22), βCH3ib (18), βCH3ir (16)
29	A′	1074		1062	1066	0.8068	0.300667	βCH3ir (49), βCH3ob (15), βCH3or (14), βCH3ib (12)
30	A″	1057	1055	1051	1051	5.9396	0.540928	βCH3or (66)
31	A′	1036		1034	1036	3.347	1.292159	βCH3or (47)
32	A′	1008		1029	1020	20.1068	8.140201	βCH3or (63), ωCO (11)
33	A′	990		984	997	0.9692	0.060308	βCH3ir (47), νCO (22)
34	A′	931	953	946	954	0.397	1.208872	βCH3ir (25), νCO (21), βCH3 or (21), βRasy (16)
35	A″	945		934	945	0.0152	0.142916	νCCsub (30), βCH3ir (23), νCO (13)
36	A′A′	799	805	798	857	1.5458	5.58439	ωCH (74), τRsym (11)
37	A″	751	748	751	749	0.0178	0.278754	νCCsub (50), βRsym (23)
38	A″	675		675	682	7.1112	0.183638	τRsym (35), ωCC (33)
39	A″	639		645	644	1.234	0.338383	βRasy (34), νCCsub (28), βRsym (15)
40	A′	627	631	630	627	0.6202	1.999952	tRasy (54), ωCC (30)
41	A″	606	603	600	605	12.885	0.14408	νCCsub (34), βCO (33), βRsym (10)
42	A″	564	556	555	563	1.0756	0.607829	τRsym (30), ωCO (29), ωCC (18), βCH3or (12)
43	A″	501	531	528	544	0.8182	0.3761	βCC (50), νCCsub (12), βCCsub (12)
44	A″		391	385	388	0.203	0.06215	βCC (37), βCO (20), νCCsub (16)
45	A′		328	318	335	0.9022	0.727572	βCCsub (49), βCC (25)
46	A′		295	302	303	5.5668	0.184802	ωCC (61), τCCCC (14)
47	A″		265	261	267	63.971	0.709247	βCC (76)
48	A″		224	208	211	2.2302	0.013186	ωCC (42), τCCH3 (27)
49	A′		174	171	176	0.466	0.514847	βCC (46), τCCH3 (15), νCH3ss (11)
50	A′		150	159	162	0.0106	0.059532	τCCH3 (43), νCH3ss (27)
51	A″			142	144	0.1146	0.008532	τCCH3 (36), νCH3ss (24), βCH3ib (13), βCH3sb (11)
52	A″			120	122	1.2076	0.391904	τCCH3 (38), βCH3ib (14)
53	A′		73	67	56	0.0236	0.409453	τCCCC (55), νCOsub (18)
54	A′			31	30	4.0968	0.148346	τCCH3 (36), βCH3ib (22), νCH3ss (19), βCH3sb (12)

[a] Abbreviations: ν, stretching; ß, in plane bending; ω, out of plane bending; τ, torsion, ss, symmetrical stretching, as, asymmetrical stretching, sc, scissoring, wa, wagging, twi, twisting, ro, rocking, ib, in-plane bending, ob, out-of-plane bending; tri, trigonal deformation, sym, symmetrical deformation, asy, asymmetric deformation, butter, butterfly, ar, aromatic, sub, substitution, vs, very strong; s, strong; ms, medium strong; w, weak; vw, very weak.
[b] Relative IR absorption intensities normalized with highest peak absorption equal to 100.
[c] Relative Raman intensities normalized to 100.
[d] Only PED contributions ≥10% are listed.

3.2.3. CO vibrations

The carbonyl stretching frequency has been most extensively studied by infrared spectroscopy [11]. This multiply bonded group is highly polar and therefore gives rise to an intense infrared absorption band. The carbon–oxygen double bond is formed by P_π–P_π bonding between carbon and oxygen. Because of the different electro negativities of carbon and oxygen atoms, the bonding electrons are not equally distributed between the two atoms. The following two resonance forms contribute to the bonding of the carbonyl group >C=O ↔ C^+—O^-. The lone pair of electrons on oxygen also determines the nature of the carbonyl group. In the present study, the band observed at 1676 cm^{-1} in FT-IR and 1666 in Ft-Raman spectrum (Table 4) was assigned to C=O stretching vibrations.

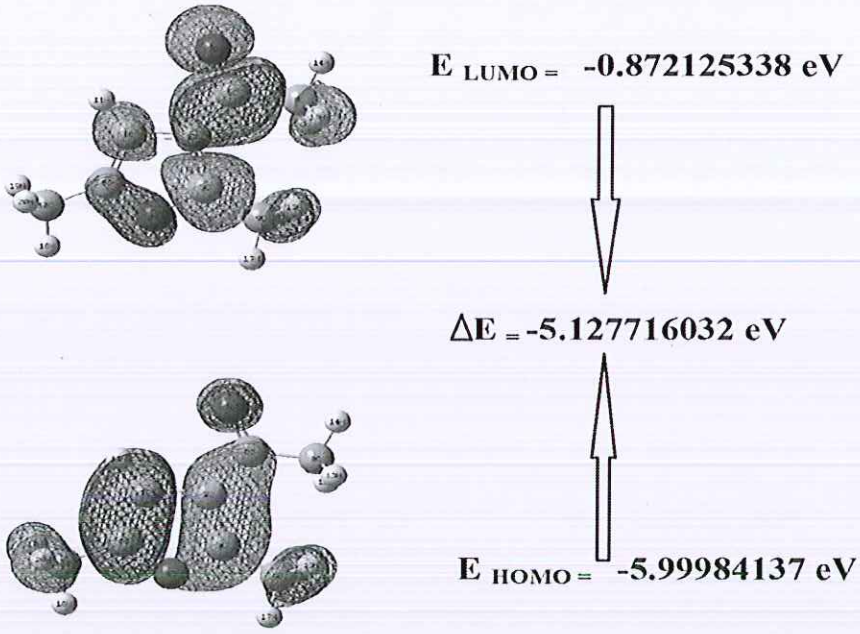

Fig. 4. The atomic orbital components of the frontier molecular orbital (HOMO-MO: 37, LUMO-MO:38) of 1-(2, 5-dimethyl-furan-3-yl)-ethanone.

3.2.4. Methyl group vibrations

For the assignments of CH3 group frequencies, basically nine fundamentals can be associated to each CH3 group namely, CH3ss, symmetrical stretch; CH3 ip, in-plane stretch (i.e., in-plane hydrogen stretching modes); CH3 ib, in-plane-bending (i.e. hydrogen deformation modes); CH3 sb, symmetric bending; CH3 ir, in-plane rocking; CH3 or, out-of-plane rocking and τCH3, twisting hydrogen bending modes. In addition to that, CH3 op, out-of-plane stretch and CH3 ob, out-of-plane bending modes of CH3 group would be expected to be depolarized symmetry species. The CH3 ss frequency is established at 2904 cm^{-1}, 2860 cm^{-1} in FT-IR, 2905 cm^{-1}, 2903 cm^{-1}, 2895 cm^{-1} in FT-Raman spectrum and CH3 ip is assigned at 2988 cm^{-1}, 2962 cm^{-1}, 2957 cm^{-1} and 2989 cm^{-1}, 2962 cm^{-1}, 2957 cm^{-1} in FT-IR and FT-Raman, respectively, for 1DF3E. These assignments are also supported by the literature [12]. The six in-plane methyl hydrogen deformation modes are also well established. The symmetrical methyl deformation mode was observed at 1420 cm^{-1}, 1402 cm^{-1}, 1232 cm^{-1} and 1416 cm^{-1}, 1221 cm^{-1} in the infrared and Raman, and in-plane-bending methyl deformation mode at 1494 cm^{-1}, 1489 cm^{-1}, 1431 cm^{-1} in FT-IR and 1511 cm^{-1} in the FT-Raman spectrum. The band at 3007 cm^{-1}, 2992 cm^{-1}, 2942 cm^{-1} and 3003 cm^{-1}, 2930 cm^{-1} in FT-IR and FT-Raman is attributed to CH3 op. Similarly the band at 1488 cm^{-1}, 1474 cm^{-1}, and 1473 cm^{-1} in FT-IR is attributed to CH3 ob. The methyl deformation modes mainly coupled with the in-plane bending vibrations. The bands obtained at 1074 cm^{-1}, 990 cm^{-1}, 931 cm^{-1} and 953 cm^{-1} in IR and Raman are assigned to CH3 in-plane and similarly the bands obtained at 1057 cm^{-1}, 1036 cm^{-1}, 1008 cm^{-1} and 1055 cm^{-1} in IR and Raman are assigned to CH3 in-plane out-of-plane rocking modes. The assignment of the band at 150 cm^{-1} in FT-Raman is attributed to methyl twisting mode.

4. Molecular orbitals

The investigation of molecular orbitals (HOMO-LUMO) is conducted to understand the distribution of electron density in HOMO and LUMO of the titled compound. The HOMO and LUMO of the investigated compound 1DF3E was showed at B3LYP/6-311++G** level of theory (Fig. 4). From Fig. 4, it is very clear that the electron density is spread majorly on oxygen donor and to a lesser extent on carbon donor in ground state (in HOMO). Upon electronic excitation one can see that electron density shifts majorly on acceptor oxygen atoms (in LUMO).

5. Conclusion

The vibrational properties of 1-(2,5-dimethyl-furan-3-yl)-etha none have been studied by FT-IR, FT-Raman spectrum and theoretical calculations have been investigated at the DFT/B3LYP/6-311++G** method. The energy at the ground state has been calculated by using above method. On the basis of the comparison between calculated and observed frequencies, assignments of fundamental vibrational modes were investigated using scaling procedure and believed to be unambiguous. The simulated and observed IR and Raman spectra agree well with the better frequency fit and intensities.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.matpr.2019.06.010.

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