



## Spectroscopic (FT-IR and UV-Vis) investigation, NBO, molecular orbital and MESP analysis of 2-(4-Isobutylphenyl) propanoic acid

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### Abstract

The FT-IR spectra of 2-(4-Isobutylphenyl) propanoic acid were recorded in the region 4000–450 cm<sup>-1</sup>. The quantum chemical calculations of geometrical structure and vibrational wavenumbers of 2-(4-isobutylphenyl) propionic acid (*abbreviated as 2IPA*) were carried out by B3LYP level with 6-311G (d,p) and 6-311++G (d,p) standard basis sets. The complete vibrational assignments of wavenumbers were performed on the basis of potential energy distribution (PED). The vibrational modes were calculated using vibrational energy distribution analysis VEDA 4 program. The UV-Vis spectrum was recorded in the region 400–200 nm. The electronic properties such as excitation energies, wavelength and oscillator's strength are calculated by TD-DFT method. The stability of the molecule has been analyzed using natural bond orbital (NBO) analysis. The thermodynamic properties the title compound zero-point vibrational energy, entropy and heat capacity have been calculated. The highest occupied molecular orbital (HOMO) and lowest unoccupied molecule orbital (LUMO) energy gap has been calculated. The molecular electrostatic potential (MESP) of the molecule were constructed.

**Keywords:** 2IPA, FT-IR, UV, HOMO-LUMO, NBO, MESP.

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## 1. Introduction

The 2-(4-Isobutylphenyl)propanoic acid belongs to a nonsteroidal anti-inflammatory drug (NSAID), it is a propionic acid derivative and nonsteroidal anti-inflammatory drug with anti-inflammatory, analgesic (pain reliever), and antipyretic (fever reducer) effects. The 2-(4-Isobutylphenyl)propanoic acid is commonly used to reduce fever and to relieve minor aches and pain from headaches, muscle aches, arthritis, toothaches, backaches, menstrual periods and the common cold. The 2-(4-Isobutylphenyl) propanoic acid is considered to be among the safest NSAIDs and is generally well tolerated but can, nevertheless, rarely cause clinically apparent and serious acute liver injury. The powder activated carbons prepared from cork waste were studied for the ibuprofen removal from liquid phase [1]. The determination of ibuprofen without interferences in complex pharmaceutical matrices such as creams and combined the dosage forms. The method involves sample pretreatment by solid-phase extraction and analytical determination by UV spectrophotometer [2]. Sagarbasha *et al.*, was studied on various chemical, functional properties and experimental studies of ibuprofen including various detection methods are potentiometric, UV-spectrophotometric, gas chromatography, HPLC and reverse-HPLC [3]. The development of a synthetic route to ibuprofen and naproxen over the last 10 years was studied and including developing methodologies [4]. Bogdan *et al.*, (2009) studied the simplicity and efficiency of this synthetic process makes it likely to satisfy the unmet need for improved ibuprofen synthesis [5]. The Asymmetric hydrogenation is a valuable methodology for chiral medicine synthesis [6]. (Kumar *et al.*, 2020) focused on recent advances and recent research on aryl propionic acid derivatives compared to medicinal chemistry [7]. Arylpropionic acid derivatives are a large and important family of non-steroidal anti-inflammatory drugs [8]. NSAIDs are often used to treat various arthritis and musculoskeletal disorders [9]. In our present investigations, the FT-IR vibrational wavenumbers were observed and the wavenumbers were theoretically computed by using quantum chemical calculations. The density functional theory B3LYP/6-311++G (d,p) calculations have been performed to support our wavenumber assignments. The FT-IR spectra of 2-(4-Isobutylphenyl)propanoic acid have been simulated using B3LYP/6-311++G (d,p) method. The NBO analysis which explains the most important orbital interactions in order to classify general structure features. The wavelength, oscillator strength, energy and natural charge analysis have been calculated. The electronic properties HOMO-LUMO energies of the compound were computed. The thermodynamic properties have been analyzed. Furthermore MESP surface of the molecule have been constructed.

## 2. FT-IR and UV-Vis measurements

The powder form of 2-(4-Isobutylphenyl) propanoic acid was procured from the leading pharmaceutical company, Sigma Aldrich, USA and used as such without further purification. The Fourier transform infrared spectrum of the title compound is measured at the room temperature recorded in the range 4000–450  $\text{cm}^{-1}$  on Bruker IFS 66V spectrophotometer using a KBr pellet technique with 4.0  $\text{cm}^{-1}$  resolution. The UV-Visible spectral measurements were carried out in ethanol using a Varian Cary 5E UV-NIR spectrometer. The spectral measurements were carried out at Sophisticated Analysis Instrumentation Facility, IIT Madras, India.

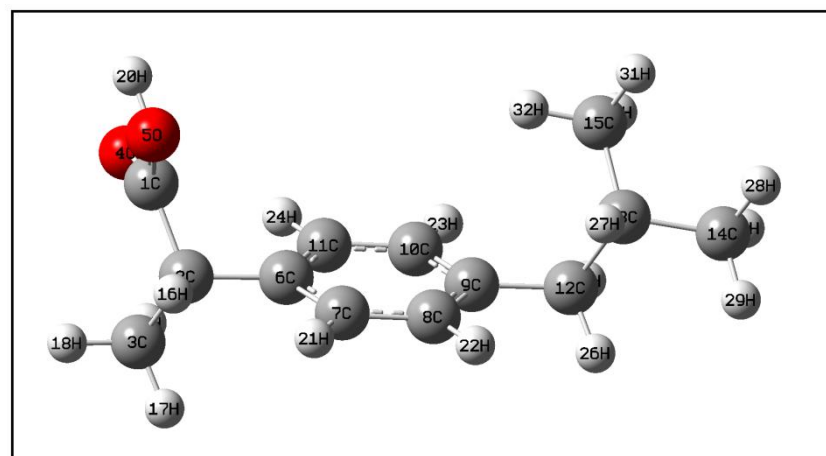
## 3. Quantum chemical calculations

All the theoretical computations were performed at density functional (DFT) theory level on a Pentium IV/1.6 GHz personal computer using the Gaussian 09 W Program package [10]. The geometries were first optimized at the B3LYP with level 6-311++G (d,p) basis set. The quantum chemical calculation has been performed using the Becke-3-Lee-Yang-Parr, (B3LYP) supplemented with the standard 6-311++G (d,p) basis set using the Gaussian 09W program to calculate the optimized geometry and vibrational wavenumbers [11,12]. The optimized structural parameters were used in the vibrational frequency calculations at DFT levels to characterize all stationary points as minima. The assignments of calculating wave numbers are aided by the animation option of Gauss View 5.0 which gives a visual presentation of the vibrational modes [13]. The natural bond orbital (NBO) analysis calculations were performed. The theoretical vibrational spectrum of 2-(4-Isobutylphenyl) propanoic acid is interpreted by means of PED using the VEDA 4 program (Jamroz, 2004) [14]. The energies, absorption wavelengths and oscillator strengths are calculated using the B3LYP method of the TD-DFT, based on the optimized structure in DMSO, ethanol and gas phase. Moreover, the changes in the thermodynamic functions (the entropy, heat capacity and enthalpy) were investigated from the vibrational frequency calculations of the title molecule. Additionally, HOMO, LUMO energy values and energy gap for 2-(4-Isobutylphenyl) propanoic acid are computed by using the B3LYP level with 6-311++G (d,p) basis set. Furthermore, MESP have been plotted in 3D by using optimized structures at B3LYP with 6-311++G (d,p) basis set.

## 4. Result and Discussion

### 4.1 Molecular structure

The optimized geometry is performed at the B3LYP level with 6-311G (d,p) and 6-311++G (d,p) basis sets of 2-(4-Isobutylphenyl) propanoic acid. The comparative optimized structural parameters such as bond angle and bond length are presented in **Table 1**. The optimized geometry of 2-(4-Isobutylphenyl) propanoic acid is shown in **Fig. 1**. The optimized molecular structure of 2-(4-Isobutylphenyl) propanoic belongs to  $C_1$  point group symmetry. The optimized structure can be compared with the experimental data (HongweiGao *et al.*, 2011)[15]. The optimized values, it is found that some of the optimized geometrical parameters are slightly deviated from the observed values, due to fact that the optimized calculations belong to molecule in the gaseous phase and the experimental results belong to molecule in the solid state. The calculated double bond length  $C_1=O_4$  and  $C_1=O_5$  were found as 1.2024, 1.3584 and 1.2044, 1.3582 Å by the B3LYP method with 6-311G (d,p) and 6-311++G (d,p) basis sets, respectively. The computed  $C_1=O_5$  bond length of the title compound value is greater than the experimental value of 1.3582 Å. The calculated  $C_1-O_4$  bond length is 1.2054 Å and  $C_2-C_6$ ,  $C_2-H_{16}$ ,  $C_{10}-C_{11}$ ,  $C_{14}-H_{30}$  bond lengths are 1.5269, 1.0914, 1.3930 and 1.0956 Å by the B3LYP method with 6-311++G (d,p) basis set which are in good agreement with the experimental values. The computed bond angle  $C_7-C_6-C_{11}$  by B3LYP with 6-311++G (d,p) basis set value  $118.0637^\circ$  is good agreement with the experimental value. The experimental  $O_4-C_1-O_5$ ,  $C_1-C_2-C_3$ ,  $C_3-C_2-C_6$  and  $C_2-C_6-C_7$  bond angles are found at  $123.4000$ ,  $111.7000$ ,  $113.1746$  and  $119.8052^\circ$  and these angles are calculated at  $122.0856$ ,  $112.4109$ ,  $114.4000$  and  $120.9000^\circ$  respectively by B3LYP level with 6-311++G (d,p) basis set.



**Fig. 1** Optimized structure of 2-(4-Isobutylphenyl) propanoic acid

**Table 1 Optimized geometrical parameters of 2-(4-Isobutylphenyl) propanoic acid**

Parameter	Calculated with B3LYP		Experimental
	6-311G(d,p)	6-311++G(d,p)	
C <sub>1</sub> -C <sub>2</sub>	1.5234	1.5236	1.5030
C <sub>1</sub> -O <sub>4</sub>	1.2024	1.2054	1.2040
C <sub>1</sub> -O <sub>5</sub>	1.3584	1.3582	1.3060
C <sub>2</sub> -C <sub>3</sub>	1.5400	1.5398	1.5000
C <sub>2</sub> -C <sub>6</sub>	1.5230	1.5269	1.5250
C <sub>2</sub> -H <sub>16</sub>	1.0915	1.0914	1.0910
C <sub>3</sub> -H <sub>17</sub>	1.0921	1.0921	1.0730
C <sub>3</sub> -H <sub>18</sub>	1.0934	1.0934	1.0530
C <sub>3</sub> -H <sub>19</sub>	1.0904	1.0904	1.0810
O <sub>5</sub> -H <sub>20</sub>	0.9690	0.9692	0.9630
C <sub>6</sub> -C <sub>7</sub>	1.3977	1.3982	1.3800
C <sub>6</sub> -C <sub>11</sub>	1.3984	1.3983	1.3740
C <sub>7</sub> -C <sub>8</sub>	1.3916	1.3923	1.3960
C <sub>7</sub> -H <sub>21</sub>	1.0852	1.0852	1.0790
C <sub>8</sub> -C <sub>9</sub>	1.3986	1.3990	1.3800
C <sub>8</sub> -H <sub>22</sub>	1.0857	1.0857	1.0650
C <sub>9</sub> -C <sub>10</sub>	1.3985	1.3988	1.3920
C <sub>9</sub> -C <sub>12</sub>	1.5125	1.5126	1.4930
C <sub>10</sub> -C <sub>11</sub>	1.3900	1.3930	1.3920
C <sub>10</sub> -H <sub>23</sub>	1.0854	1.0855	1.0410
C <sub>11</sub> -H <sub>24</sub>	1.0836	1.0837	1.1030
C <sub>12</sub> -C <sub>13</sub>	1.5489	1.5487	1.5290
C <sub>12</sub> -H <sub>25</sub>	1.096	1.0961	1.1020
C <sub>12</sub> -H <sub>26</sub>	1.0962	1.0963	1.1010
C <sub>13</sub> -C <sub>14</sub>	1.5343	1.5344	1.5080
C <sub>13</sub> -C <sub>15</sub>	1.5336	1.5336	1.5190
C <sub>13</sub> -H <sub>27</sub>	1.0976	1.0976	1.0850
C <sub>14</sub> -H <sub>28</sub>	1.0937	1.0938	1.0610
C <sub>14</sub> -H <sub>29</sub>	1.0941	1.0942	1.0620
C <sub>14</sub> -H <sub>30</sub>	1.0955	1.0956	1.0970
C <sub>15</sub> -H <sub>31</sub>	1.0937	1.0938	1.0670
C <sub>15</sub> -H <sub>32</sub>	1.0923	1.0924	1.0990
C <sub>15</sub> -H <sub>33</sub>	1.0959	1.0961	1.0440

Bond angle (°)			
C <sub>2</sub> -C <sub>1</sub> -O <sub>4</sub>	125.1735	125.0985	121.1000
C <sub>2</sub> -C <sub>1</sub> -O <sub>5</sub>	112.6989	112.8142	115.4000
O <sub>4</sub> -C <sub>1</sub> -O <sub>5</sub>	122.1265	122.0856	123.4000
C <sub>1</sub> -C <sub>2</sub> -C <sub>3</sub>	112.4674	112.4109	111.7000
C <sub>1</sub> -C <sub>2</sub> -C <sub>6</sub>	110.4712	110.2114	106.7000
C <sub>1</sub> -C <sub>2</sub> -H <sub>16</sub>	104.0747	104.1574	0.0000
C <sub>3</sub> -C <sub>2</sub> -C <sub>6</sub>	112.7046	113.1746	114.4000
C <sub>3</sub> -C <sub>2</sub> -16	109.0888	108.9163	-
C <sub>6</sub> -C <sub>2</sub> -16	107.5483	107.4476	-
C <sub>2</sub> -C <sub>3</sub> -17	109.5835	109.5001	-
C <sub>2</sub> -C <sub>3</sub> -H <sub>18</sub>	110.985	110.8719	-
C <sub>2</sub> -C <sub>3</sub> -H <sub>19</sub>	111.3443	111.6125	-
H <sub>17</sub> -C <sub>3</sub> -H <sub>18</sub>	108.3154	108.3139	-
H <sub>17</sub> -C <sub>3</sub> -H <sub>19</sub>	108.4033	108.4018	-
H <sub>18</sub> -C <sub>3</sub> -H <sub>19</sub>	108.1185	108.0460	-
C <sub>1</sub> -O <sub>5</sub> -H <sub>20</sub>	106.2776	106.9406	-
C <sub>2</sub> -C <sub>6</sub> -C <sub>7</sub>	119.9156	119.8052	120.9000
C <sub>2</sub> -C <sub>6</sub> -C <sub>11</sub>	121.9867	122.1289	120.9000
C <sub>7</sub> -C <sub>6</sub> -C <sub>11</sub>	118.0894	118.0637	118.2000
C <sub>6</sub> -C <sub>7</sub> -C <sub>8</sub>	121.0138	121.0259	120.7000
C <sub>6</sub> -C <sub>7</sub> -H <sub>21</sub>	119.4686	119.4946	-
C <sub>8</sub> -C <sub>7</sub> -H <sub>21</sub>	119.5168	119.4789	-
C <sub>7</sub> -C <sub>8</sub> -C <sub>9</sub>	121.1493	121.1632	120.7000
C <sub>7</sub> -C <sub>8</sub> -H <sub>22</sub>	119.2812	119.2059	-
C <sub>9</sub> -C <sub>8</sub> -H <sub>22</sub>	119.569	119.6303	-
C <sub>8</sub> -C <sub>9</sub> -C <sub>10</sub>	117.6206	117.5857	118.0000
C <sub>8</sub> -C <sub>9</sub> -C <sub>12</sub>	120.784	120.8124	121.8000
C <sub>10</sub> -C <sub>9</sub> -C <sub>12</sub>	121.5924	121.5997	120.2000
C <sub>9</sub> -C <sub>10</sub> -C <sub>11</sub>	121.4376	121.4504	120.7000
C <sub>9</sub> -C <sub>10</sub> -H <sub>23</sub>	119.3012	119.3460	-
C <sub>11</sub> -C <sub>10</sub> -H <sub>23</sub>	119.2611	119.2037	-
C <sub>6</sub> -C <sub>11</sub> -C <sub>10</sub>	120.6882	120.7098	121.6000
C <sub>6</sub> -C <sub>11</sub> -H <sub>24</sub>	119.8155	119.9774	-
C <sub>10</sub> -C <sub>11</sub> -H <sub>24</sub>	119.4931	119.3106	-
C <sub>9</sub> -C <sub>12</sub> -C <sub>13</sub>	114.7364	114.7850	113.9000
C <sub>9</sub> -C <sub>12</sub> -H <sub>25</sub>	108.9878	108.9953	-

C <sub>9</sub> -C <sub>12</sub> -H <sub>26</sub>	109.4714	109.4198	-
C <sub>13</sub> -C <sub>12</sub> -H <sub>25</sub>	108.2647	108.2692	-
C <sub>13</sub> -C <sub>12</sub> -H <sub>26</sub>	108.6599	108.6510	-
H <sub>25</sub> -C <sub>12</sub> -H <sub>26</sub>	106.3905	106.3877	-
C <sub>12</sub> -C <sub>13</sub> -C <sub>14</sub>	110.2733	110.2419	110.1000
C <sub>12</sub> -C <sub>13</sub> -C <sub>15</sub>	112.0781	112.0812	111.5000
C <sub>12</sub> -C <sub>13</sub> -H <sub>27</sub>	107.4012	107.4318	-
C <sub>14</sub> -C <sub>13</sub> -C <sub>15</sub>	111.0007	111.0281	115.5000
C <sub>14</sub> -C <sub>13</sub> -H <sub>27</sub>	107.9951	107.9619	-
C <sub>15</sub> -C <sub>13</sub> -H <sub>27</sub>	107.9108	107.9138	-
C <sub>13</sub> -H <sub>14</sub> -H <sub>28</sub>	111.127	111.1157	-
C <sub>13</sub> -C <sub>14</sub> -H <sub>29</sub>	111.4985	111.5028	-
C <sub>13</sub> -C <sub>14</sub> -H <sub>30</sub>	110.8673	110.9033	-
H <sub>28</sub> -C <sub>14</sub> -H <sub>29</sub>	107.851	107.8367	-
H <sub>28</sub> -C <sub>14</sub> -H <sub>30</sub>	107.5864	107.5872	-
H <sub>29</sub> -C <sub>14</sub> -H <sub>30</sub>	107.7398	107.7229	-
C <sub>13</sub> -C <sub>15</sub> -H <sub>31</sub>	110.8449	110.8425	-
C <sub>13</sub> -C <sub>15</sub> -H <sub>32</sub>	111.6825	111.7080	-
C <sub>13</sub> -C <sub>15</sub> -H <sub>33</sub>	110.7742	110.8065	-
H <sub>31</sub> -C <sub>15</sub> -H <sub>32</sub>	107.8892	107.8654	-
H <sub>31</sub> -C <sub>15</sub> -H <sub>33</sub>	107.6173	107.6032	-
H <sub>32</sub> -C <sub>15</sub> -H <sub>33</sub>	107.8712	107.8504	-

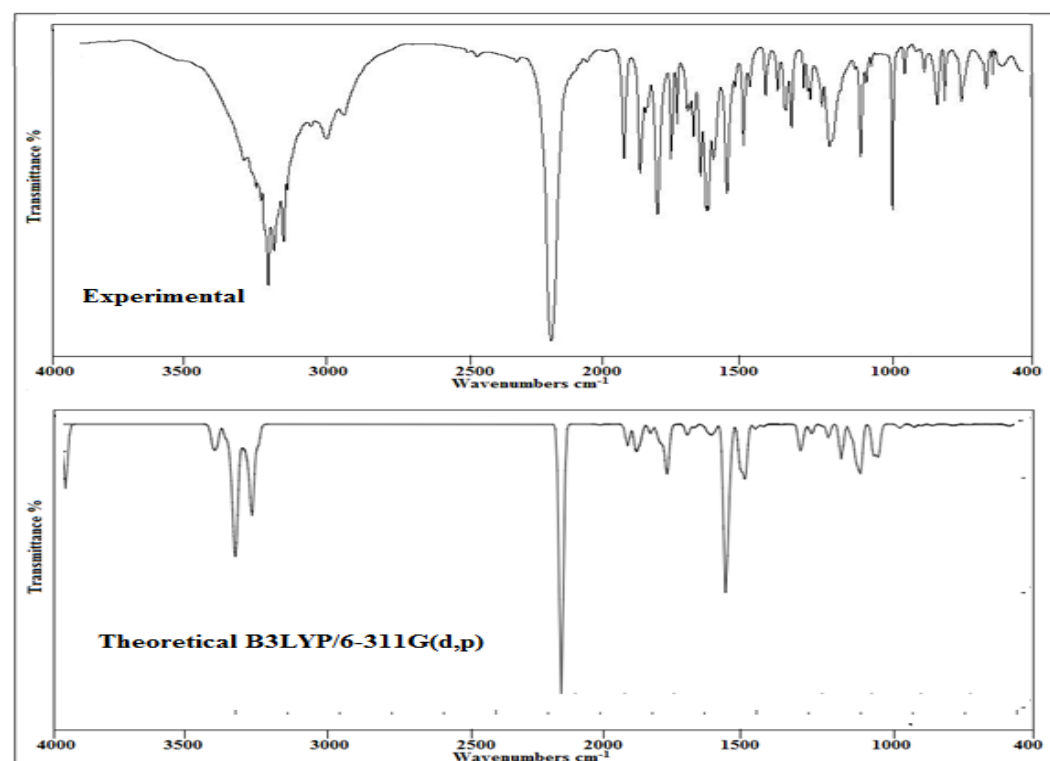
## 4.2 Analysis of vibrational spectra

The title molecule consists of 33 atoms, and so they have 93 normal modes of fundamental vibrations. The observed and simulated FT-IR spectrum is shown in **Fig. 2**. The harmonic vibrational frequencies calculated for 2-(4-Isobutylphenyl) propanoic acid at B3LYP level with 6-311G (d,p) and 6-311++G (d,p) basis sets, have been collected in **Table 2**. The maximum number of values determined by B3LYP level with 6-311++G (d,p) basis set, is in good agreement with the observed values. The computed frequencies are slightly higher than the experimental values for the majority of the normal modes. Two factors may be the reason for the discrepancies between the observed and calculated spectra of this compound. The first is the influence of the environment and the second one is the fact that the observed value is anharmonic frequency while the computed value is a harmonic frequency. The calculated harmonic wavenumbers are usually higher than the

corresponding observed quantities because of the combination of electron correlation effects and the basis set deficiencies.

#### 4.2.1 O-H Vibration frequency

In the title molecules contain O-H stretching frequency occurred in range 3200–3550  $\text{cm}^{-1}$ [16]. In the present work calculated O-H vibrational frequency range 3557, 3555  $\text{cm}^{-1}$  with 100% contribution in PED carried out two methods 6-311G (d,p), 6-311++G (d,p) and the FT-IR spectra observed at 3554  $\text{cm}^{-1}$ , theoretical 6-311++G (d,p) basis set good agreement with experimental data respectively.



**Fig. 2 FT-IR spectra of 2-(4-Isobutylphenyl) propanoic acid**

#### 4.2.2 Carbonyl group oscillating frequency

The carbonyl group of C=O frequency in benzene ring assigned at 1685–1660  $\text{cm}^{-1}$ [17]. In the current investigation theoretically calculated carbon=oxygen banding range at 1689,1683  $\text{cm}^{-1}$  with contribution PED value 86 %, 6-311++G(d,p) method as well as merge with FT-IR range occur strong intensity at 1655  $\text{cm}^{-1}$  respectively.

#### 4.2.3 C-H stretching frequency

Normally, the stretching wavenumber of C-H band given multiple peaks occur area 3100–3000  $\text{cm}^{-1}$ [18]. In the present study experimental peak was observed at 3005, 3056,



3075  $\text{cm}^{-1}$  and the corresponding calculated stretching wavenumber assigned at 3012, 3060, 3080  $\text{cm}^{-1}$  by 6-311G(d,p), 3002, 3052, 3072  $\text{cm}^{-1}$  by 6-311++G(d,p) both methods are good agreement with literature values successively.

**Table 2 Vibrational assignments of 2-(4-Isobutylphenyl) propanoic acid**

Experimental wavenumber ( $\text{cm}^{-1}$ )	Calculated wavenumber ( $\text{cm}^{-1}$ ) B3LYP		Vibrational assignment (PED %)
	6-311G(d,p)	6-311++G(d,p)	
3554	3557	3555	$\nu$ OH(100)
	3188	3187	$\nu$ CH <sub>2</sub> (100)
	3169	3170	$\nu$ CH <sub>2</sub> (95)
	3158	3159	$\nu$ CH <sub>2</sub> (90)
	3151	3152	$\nu$ CH <sub>2</sub> (66)
3120	3130	3124	$\nu$ CH <sub>3</sub> (73)
3098	3105	3100	$\nu$ CH <sub>2</sub> (50)
3090	3098	3092	$\nu$ CH <sub>2</sub> (77)
3065	3085	3080	$\nu$ CH <sub>2</sub> (33)
3075	3080	3077	$\nu$ CH(94)
	3077	3078	$\nu$ CH(28)
	3073	3071	$\nu$ CH(30)
3056	3060	3052	$\nu$ CH(51)
	3037	3037	$\nu$ CH(49)
	3021	3019	$\nu$ CH(30)
	3014	3012	$\nu$ CH(33)
	3013	3011	$\nu$ CH(18)
3005	3012	3002	$\nu$ CH(87)
	1827	1805	$\nu$ CC(29)
1655	1689	1683	$\nu$ OC(86)
1620	1630	1625	$\nu$ CC(11)+ $\delta$ CCC(11)
	1543	1542	$\delta$ HCC(26)
	1516	1511	$\delta$ HCH(23)
	1506	1504	$\delta$ HCH(31)
	1502	1501	$\delta$ HCH(54)
	1498	1496	$\delta$ HCH(29)
	1496	1495	$\delta$ HCH(38)
	1491	1490	$\delta$ HCH(25)

	1485	1484	$\delta$ HCH(38)
1470	1454	1451	$\nu$ CC(12)+ $\delta$ HCC(10)
	1422	1421	$\delta$ HCH(16)
	1415	1414	$\delta$ HCH(10)
	1402	1401	$\delta$ HCH(19)
	1374	1374	$\delta$ HCC(10)+ $\tau$ HCCC(14)
1350	1370	1368	$\tau$ CCCH(24)
	1367	1366	$\delta$ HCC(22)
	1351	1346	$\delta$ HCCC(13)
	1342	1342	$\delta$ HCCC(48)
1315	1336	1335	$\delta$ HOC(28)
	1316	1316	$\delta$ HCC(34)+ $\tau$ HCCC(15)
1273	1294	1295	$\delta$ HCC(19)+ $\nu$ CC(11)
	1245	1245	$\delta$ HCC(16)+ $\tau$ HCCC(12)
	1228	1227	$\nu$ CC(29)
	1216	1215	$\delta$ HCC(15)+ $\nu$ CC(16)
1227	1209	1208	$\nu$ CC(11)
	1189	1187	$\nu$ CC(11)+ $\tau$ HCCC(13)
	1188	1185	$\nu$ OC(17)
	1148	1148	$\delta$ HCC(17)+ $\nu$ CC(13)
	1134	1133	$\nu$ CC(21)
	1107	1107	$\delta$ HCC(21)
1059	1086	1084	$\delta$ HCC(10)+ $\nu$ CC(19)
1045	1057	1056	$\nu$ CC(23)+ $\tau$ HCCC(27)
	1037	1037	$\delta$ CCC(16)
	995	996	$\nu$ OC(18)+ $\tau$ HCCC(14)
	980	984	$\tau$ HCCC(34)
	971	969	$\tau$ HCCC(22)+ $\tau$ CCCC(11)
	966	966	$\nu$ CC(17)+ $\tau$ HCCC(10)
	951	951	$\nu$ CC(30)
914	932	931	$\tau$ HCCC(25)
873	891	892	$\tau$ HCCC(21)
	868	867	$\tau$ HCCC(11)
829	853	850	$\tau$ HCCC(20)
	851	849	$\nu$ CC(10)
	830	829	$\nu$ CC(13)

	818	817	$\gamma$ OCOC(31)
	800	798	$\nu$ CC(12)
	750	746	$\tau$ HOCC(12)+ $\gamma$ CCCC(11)
	724	721	$\delta$ CCC(10)
	660	658	$\delta$ CCC(25)
	640	635	$\tau$ HOCC(12)+ $\gamma$ CCCC(11)
	611	608	$\tau$ HOCC(37)
	582	581	$\tau$ HOCC(16)
	554	550	$\gamma$ CCCC(19)
	450	450	$\nu$ CC(14)
	425	425	$\gamma$ CCCC(11)
	418	418	$\tau$ CCCC(31)
	403	404	$\delta$ CCC(29)
	381	383	$\delta$ CCC(30)
	343	343	$\delta$ CCC(15)
	312	315	$\delta$ OCC(18)+ $\delta$ CCC(11)
	295	295	$\delta$ CCC(33)
	250	251	$\delta$ OCC(10)+ $\delta$ CCC(16)+ $\tau$ HCCC(11)
	242	246	$\delta$ CCC(12)
	237	231	$\tau$ HCCC(12)
	224	227	$\tau$ HCCC(23)
	196	195	$\delta$ CCC(13)+ $\gamma$ CCCC(14)
	161	164	$\delta$ CCC(28)+ $\gamma$ CCCC(14)
	112	111	$\delta$ CCC(18)+ $\gamma$ CCCC(11)
	69	69	$\tau$ OCCC(10)+ $\tau$ CCCC(46)
	53	53	$\tau$ OCCC(10)+ $\tau$ CCCC(40)
	46	48	$\tau$ CCCC(29)
	39	40	$\tau$ CCCC(22)+ $\gamma$ CCCC(17)
	22	24	$\gamma$ CCCC(11)

#### 4.2.4 CH<sub>2</sub> Vibrations

The CH<sub>2</sub> stretching vibration [19]. In the present investigation CH<sub>2</sub> frequency calculated range at 3085, 3098, 3105 cm<sup>-1</sup> by 6-311G(d,p) and 3080, 3092, 3100 cm<sup>-1</sup> by 6-311++G(d,p) with mixed contribution PED values 33%, 77%, 50% are corresponding FT-IR spectra data 3065, 3090, 3098 cm<sup>-1</sup> are good correlation respectively.

#### 4.2.5 CH<sub>3</sub> Vibrations

The CH<sub>3</sub> stretching frequency previously observed at 3100-3000 cm<sup>-1</sup>. In the present investigation of methyl group in the title molecules is observed to vibrate within the expected range 3130, 3124 cm<sup>-1</sup> calculated by two methods (6-311G(d,p), 6-311++G(d,p)) with PED contribution 73% and the experimental spectra observed region at 3120 cm<sup>-1</sup> medium intensity. The FT-IR wavenumber frequency compared with density functional calculation is as well as coincides.

#### 4.2.6 C-C Vibrations

Vibrational modes of C-C band were observed at 1640-1200 cm<sup>-1</sup>[20]. In the title molecules theoretical prediction of C-C stretching frequency 1209, 1454, 1630 cm<sup>-1</sup> carried out 6-311G(d,p) and 1208, 1451, 1625 cm<sup>-1</sup> carried out 6-311++G(d,p) are compared with FT-IR spectra 1227, 1470, 1620 cm<sup>-1</sup>. The experimental values are good agreement with two theoretical methods successively.

#### 4.3 Natural Bond Orbital (NBO) study

The Natural Bond Orbital calculation were performed at DFT/B3LYP with 6-311++G(d, p) basis set using Gaussian 09 W program. NBO analysis is used to find the interaction between the bond orbitals, bond bending effect, electron delocalization and intermolecular charge transfer. Therefore, Natural Bond Orbital theory is a valuable complement to the energetic and structural data. A large number of stabilizing orbital interactions are calculated for 2-(4-Isobutylphenyl)propanoic acid molecule. For the each donor (i) and acceptor (j) the stabilization energy E(2) associated with the delocalization i→j is determined as

$$E(2) = \Delta E_{ij} = q_i \frac{F(i,j)^2}{\epsilon_j - \epsilon_i}$$

$\epsilon_j, \epsilon_i$  the diagonal elements,  $q_i$  is the donor orbital occupancy and  $F(i, j)$  is the off diagonal Natural Bond Orbital Fock matrix element. The delocalization of the electron density between the occupied Lewis-type (bonding or lone pair) Natural Bond Orbital and formally unoccupied non-Lewis (ant bonding or Rydberg) Natural Bond Orbitals correspond to a stabilizing donor-acceptor interaction. The important interactions between the 'filled' Lewis-type NBOs and 'empty' Non-Lewis NBOs according to second order perturbation energy values, E(2) of 2-(4-Isobutylphenyl)propanoic acid is given in **Table 3**. The most important

interactions in the title molecule having lone pair LP(2) O<sub>5</sub> with that of anti-bonding C<sub>1</sub>-O<sub>4</sub> and the lone pair LP(2) O<sub>4</sub> with that of anti-bonding C<sub>1</sub>-O<sub>5</sub> and results the stabilization of 42.850 kJ/mol and 37.060 kJ/mol respectively[24, 25]. The maximum energy transfer occurs from LP(2) O<sub>5</sub> and LP(2) O<sub>4</sub> to C<sub>1</sub>-O<sub>4</sub> and C<sub>1</sub>-O<sub>5</sub>. In 2-(4-Isobutylphenyl)propanoic acid, the interactions LP(2)O<sub>5</sub>→ $\pi^*(C_1-O_4)$  have the highest E(2) value of 42.850 kJ/mol.

**Table 3 NBO analysis of 2-(4-Isobutylphenyl) propanoic acid**

Type	Donor (i)	Occupancy (e)	Type	Acceptor (j)	Occupancy (e)	E <sup>a</sup> (2) (kcal/mol)	E(j)-E(i) <sup>b</sup> (a.u)	F(i, j) <sup>c</sup> (a.u)
$\pi$	C <sub>6</sub> -C <sub>11</sub>	1.65588	$\pi^*$	C <sub>7</sub> -C <sub>8</sub>	0.32762	20.540	0.280	0.068
$\pi$	C <sub>6</sub> -C <sub>11</sub>	1.65588	$\pi^*$	C <sub>9</sub> -C <sub>10</sub>	0.34367	19.640	0.290	0.067
$\pi$	C <sub>7</sub> -C <sub>8</sub>	1.67075	$\pi^*$	C <sub>6</sub> -C <sub>11</sub>	0.35699	20.370	0.290	0.069
$\pi$	C <sub>7</sub> -C <sub>8</sub>	1.67075	$\pi^*$	C <sub>9</sub> -C <sub>10</sub>	0.34367	21.040	0.290	0.070
$\pi$	C <sub>9</sub> -C <sub>10</sub>	1.64321	$\pi^*$	C <sub>6</sub> -C <sub>11</sub>	0.35699	21.890	0.280	0.070
$\pi$	C <sub>9</sub> -C <sub>10</sub>	1.64321	$\pi^*$	C <sub>7</sub> -C <sub>8</sub>	0.32762	19.800	0.280	0.069
LP(2)	O <sub>4</sub>	1.84953	$\sigma^*$	C <sub>1</sub> -C <sub>2</sub>	0.06887	17.460	0.640	0.096
LP(2)	O <sub>4</sub>	1.84953	$\sigma^*$	C <sub>1</sub> -O <sub>5</sub>	0.10330	37.060	0.600	0.130
LP(2)	O <sub>5</sub>	1.82875	$\pi^*$	C <sub>1</sub> -O <sub>4</sub>	0.19664	42.850	0.350	0.110

E (2)<sup>a</sup> means energy of hyper conjugative interaction.

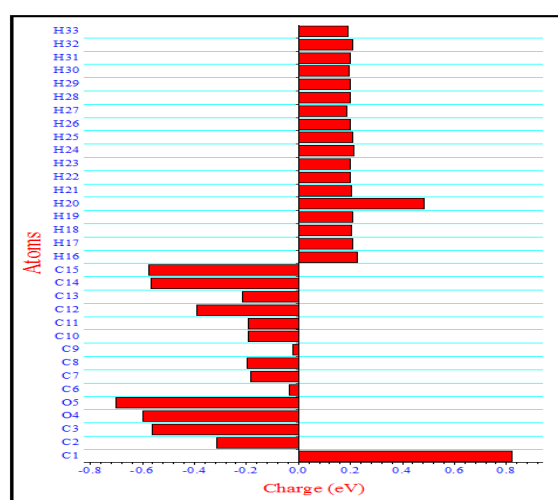
<sup>b</sup> Energy difference between donor and acceptor i and j NBO orbitals.

F(i,j)<sup>c</sup> is the Fock matrix element between i and j NBO orbitals.

#### 4.4 Natural atomic charge analysis

The natural atomic charges of 2-(4-Isobutylphenyl) propanoic acid calculated by Natural Bond Orbital analysis by B3LYP/6-311++G(d,p) method were listed in **Table 4**. The illustration of natural atomic charge plot is shown in **Fig. 3**. The natural atomic charge affects the polarizability, dipole moment, electronic structure and other properties of molecular system. The natural atomic charge distributions over the atoms suggest the formation of acceptor and donor pairs involving the charge transfer in the molecule. The electronegative O<sub>4</sub> and O<sub>5</sub> atoms of compound 2-(4-Isobutylphenyl) propanoic acid have negative charge values. The natural atomic charges of the mentioned atoms were calculated as -0.59638 and -0.70114 eV respectively. The C<sub>1</sub> and H<sub>20</sub> atoms bounded to the mentioned electronegative atoms in the molecule under study have positive charge values. The values of the positive charges of the mentioned atoms were found as 0.82310 and 0.48422 eV

respectively. Therefore the C<sub>1</sub> atom surrounded with two electronegative O<sub>4</sub> and O<sub>5</sub> atoms have the highest positive charge values. The maximum atomic charge is obtained for C<sub>1</sub> atom for when compared to other atoms. This is due to the attachment of negatively charged oxygen atoms. All the hydrogen atoms are positive charges. The negative charged lone pair oxygen O<sub>4</sub> and O<sub>5</sub> shows that charge is transferred from O to C (O<sub>4</sub>→C<sub>1</sub>) and (O<sub>5</sub>→C<sub>1</sub>). The maximum negative and positive charge is represented in O<sub>5</sub> and C<sub>1</sub> atoms respectively [26]. The charge distribution of 2-(4-Isobutylphenyl) propanoic acid shows that the carbon C<sub>1</sub> atoms is attached with oxygen O<sub>4</sub> and O<sub>5</sub> atoms of the ring is positive because of the electron withdrawing nature of the O atoms, whereas the remaining carbon atoms are negatively charged.



**Fig. 3** Natural charge distribution of 2-(4-Isobutylphenyl) propanoic acid

**Table 4** The natural charge analysis of 2-(4-Isobutylphenyl) propanoic acid

Atoms	Charges (eV)	Atoms	Charges (eV)
C1	0.82310	H18	0.20414
C2	-0.31461	H19	0.20903
C3	-0.56182	H20	0.48422
O4	-0.59638	H21	0.20385
O5	-0.70114	H22	0.20150
C6	-0.03721	H23	0.20155
C7	-0.18551	H24	0.21251
C8	-0.19502	H25	0.20758
C9	-0.02380	H26	0.19822
C10	-0.19213	H27	0.18454
C11	-0.19395	H28	0.20069
C12	-0.39285	H29	0.19749
C13	-0.21489	H30	0.19309
C14	-0.56804	H31	0.19983
C15	-0.57555	H32	0.20839
H16	0.22491	H33	0.19070
H17	0.20754		

#### 4.5 Thermodynamic parameters

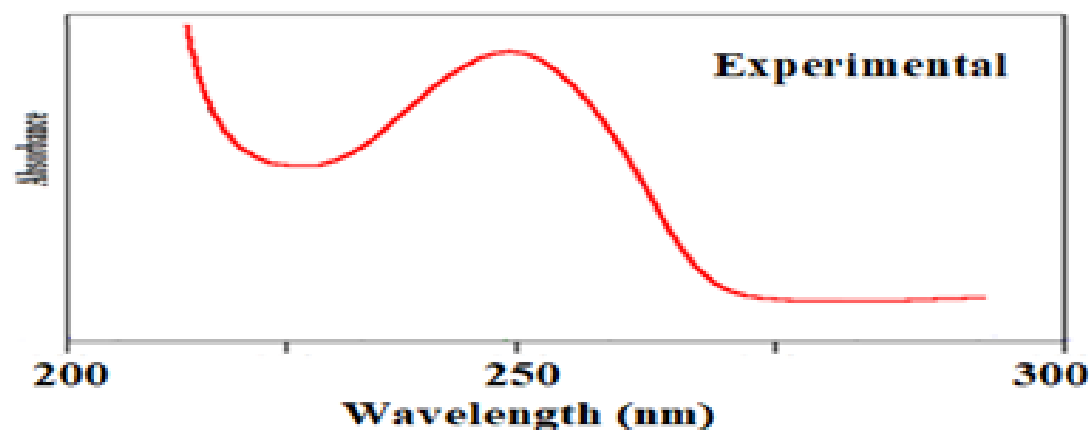
Thermodynamic properties like zero-point vibrational energy (ZPVEs), heat capacity, thermal energy, rotational constants, entropy and dipole moment of the title compound have also been calculated at B3LYP level with 6-311G (d,p) and 6-311++G (d,p) basis sets and they are presented in **Table 5**. The thermodynamic parameters supply helpful and extra information about the 2-(4-Isobutylphenyl)propanoic acid. The variation in Zero-Point Vibrational Energies (ZPVEs) seems to be important [27, 28]. The Zero-Point Vibrational Energies is lower in the B3LYP/6-311++G (d,p) than by B3LYP/6-311G (d,p) method. The entropy and specific heat capacity were calculated and their values were found to be the highest values for B3LYP/6-311++G (d,p) but the smallest values were obtained by the B3LYP/6-311G (d,p) method. The minimum value of thermal energy was calculated as 187.743 kJ/mol by B3LYP/6-311++G (d,p) whereas the maximum value one was calculated as 187.885 kJ/mol by the B3LYP/6-311G (d,p) for 2-(4-Isobutylphenyl)propanoic acid molecule.

**Table 5 Thermodynamic parameters of 2-(4-Isobutylphenyl) propanoic acid**

Parameter	B3LYP/6-311G(d,p)	B3LYP/6-311++G(d,p)
Zero-Point		
Vibrational Energy (kJ/mol)	178.007300	177.865030
Rotational constant (GHz)	1.359150	1.348520
	0.253740	0.254160
	0.243000	0.244210
Thermal Energy (kJ/mol)		
Total	187.885000	187.743000
Translational	0.889000	0.889000
Rotational	0.889000	0.889000
Vibrational	186.107000	185.965000
Heat capacity constant (cal/mol <sup>-1</sup> K <sup>-1</sup> )		
Total	58.942000	59.009000
Translational	2.981000	2.981000
Rotational	2.981000	2.981000
Vibrational	52.980000	53.047000
Entropy (cal/mol <sup>-1</sup> K <sup>-1</sup> )		
Total	129.190000	129.390000
Translational	41.874000	41.874000
Rotational	32.617000	32.618000
Vibrational	54.892000	54.698000

#### 4.6 UV-Visible spectral analysis

The experimental spectrum of the title compound in ethanol was recorded within the range 400–200 nm and shown in **Fig. 4**. The UV-Visible spectral analysis of 2-(4-Isobutylphenyl) propanoic acid has been investigated in ethanol, DMSO and gas phase for theoretical calculation. The calculated electronic excitation energies (E), oscillator strengths (f) and absorption wavelengths ( $\lambda$ ) are compared with the experimental wavelength. The calculated time dependent density functional theory TD-DFT/6-311++G (d,p) approach as this method produced good coherent with the experimental data [29, 30]. The computed absorption maxima values have been found to be 241.41, 230.35 and 216.89 nm for gas phase and 241.32, 239.36 and 210.32 nm for DMSO and 243.31, 239.24 and 212.37 nm for ethanol and presented in **Table 6**. The B3LYP/6-311++G (d,p) calculated absorption wavelength at 243.19 nm is in good agreement with experimental absorption wavelength at 241.00 nm in the UV-Vis spectrum.



**Fig. 4. Experimental Electron Transition of 2-(4-Isobutylphenyl) propanoic acid**

**Table 6 Wavelength, oscillatory strength and energy of 2-(4-Isobutylphenyl) propanoic acid**

Calculated with B3LYP/6-311++G(d,p)									Exp
Gas phase			DMSO			Ethanol			
$\lambda_{\max}$ (nm)	E (ev)	f	$\lambda_{\max}$ (nm)	E (ev)	f	$\lambda_{\max}$ (nm)	E (ev)	f	$\lambda_{\max}$ (nm)
241.4100	5.1147	0.0006	241.3200	5.1166	0.0062	243.3100	5.1167	0.0056	243.0000
230.3500	5.2457	0.1560	239.3600	5.2016	0.1982	239.2400	5.2042	0.1939	-
216.89 nm	5.6903	0.0055	210.3200	5.7850	0.0142	212.3700	5.7835	0.0137	-

#### 4.7 Analysis of frontier molecular orbitals



The Highest Occupied Molecular Orbitals and Lowest Unoccupied Molecular Orbitals are named as Frontier molecular orbital's (FMOs). The atomic orbital compositions of the frontier molecular orbital are shown in **Fig. 5**. The highest occupied molecular orbitals (HOMO) and lowest unoccupied molecular orbital (LUMO) energy gap of 2-(4-Isobutylphenyl) propanoic acid was calculated using B3LYP level with 6-311++G (d,p) basis set and is presented in **Table 7** [31]. The energy values of HOMO and LUMO levels for 2-(4-Isobutylphenyl) propanoic acid molecule are 6.6856 and 0.8019 eV by B3LYP with 6-311++G (d,p) basis set respectively. The HOMO-LUMO energy difference is 5.8837 eV. The positive and negative phase is represented in red and green color respectively[32, 33]. A large HOMO-LUMO energy gap implies high stability and low reactivity. The small HOMO-LUMO energy gap means a low stability and high reactivity.

The most widely used theory by the chemists is the frontier molecular orbital theory. It is important that the Ionization potential (I), Electrophilicity ( $\omega$ ), Electron affinity (A), Electronegativity ( $\chi$ ), Hardness ( $\eta$ ), Softness (S) and Chemical potential ( $\mu$ ) be put into a MO framework. The quantum chemical parameters of the molecule are presented in **Table 7**. We focus on the HOMO and LUMO energies in order to determine the interesting molecular properties and chemical quantities. In simple molecular orbital theory approaches, the Highest Occupied Molecular Orbitals energy is related to the ionization potential (I) and the Lowest Unoccupied Molecular Orbitals energy has been used to estimate the electron affinity (A) respectively.

The Ionization potential of the 2-(4-Isobutylphenyl) propanoic acid is  $(I) = -E_{\text{HOMO}}$

The electrophilicity index of the 2-(4-Isobutylphenyl) propanoic acid is  $(\omega) = \mu^2/2\eta$ .

The Electron affinity of the 2-(4-Isobutylphenyl) propanoic acid is  $(A) = -E_{\text{LUMO}}$ .

The electronegativity of the 2-(4-Isobutylphenyl) propanoic acid is  $(\chi) = (I+A)/2$ .

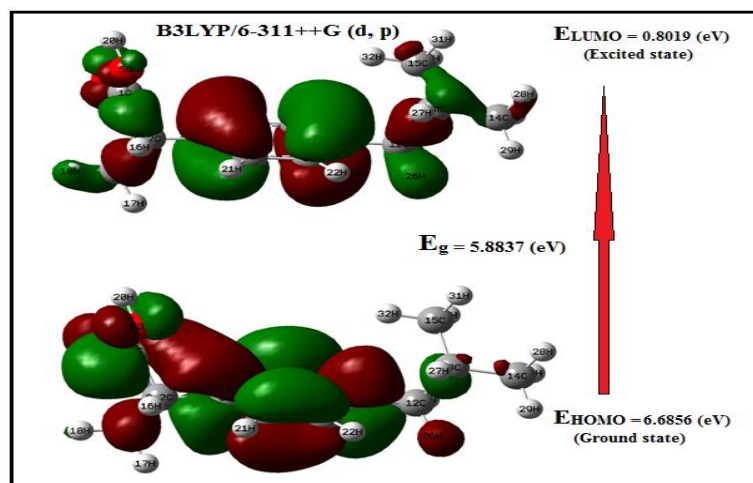
The absolute hardness of the 2-(4-Isobutylphenyl) propanoic acid is  $(\eta) = (I-A)/2$ .

The softness is the inverse of the hardness of the 2-(4-Isobutylphenyl) propanoic acid is  $(S) = 1/\eta$ .

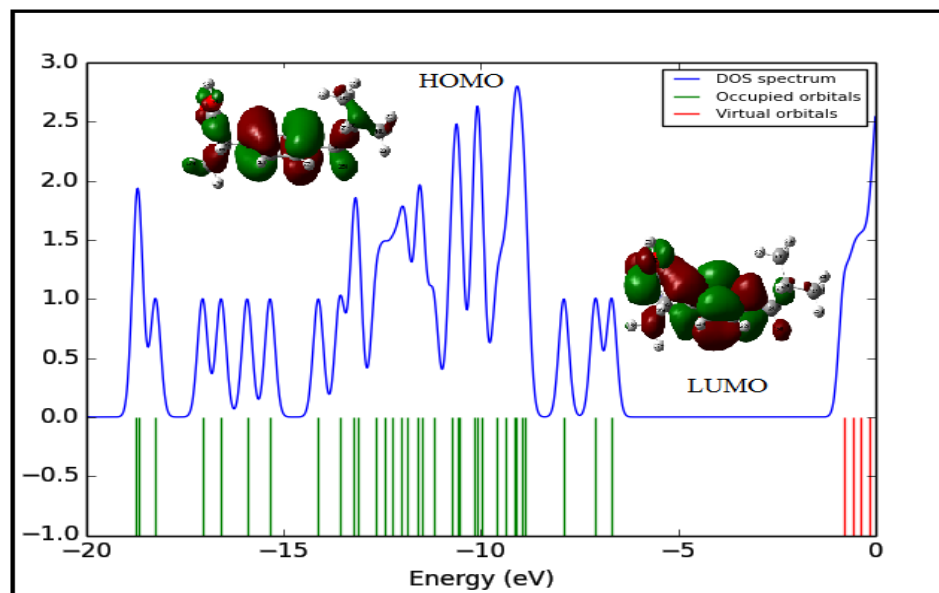
The chemical potential of the 2-(4-Isobutylphenyl) propanoic acid is  $(\mu) = -(I+A)/2$ .

The values of ionization potential, electrophilicity, Electron affinity, electronegativity, absolute hardness, softness and chemical potential are -6.6856, -2.3820, -0.8019, -3.7437, -2.9418, -0.3399, and 3.7437eV calculated at B3LYP level with 6-311++G (d,p) basis set respectively. The gauss-Sum 2.2 program was used to compute the group contributions to the

molecular orbital (Highest Occupied Molecular Orbitals and Lowest Unoccupied Molecular Orbitals) and to prepare the Density of States (DOS) spectrum as shown in **Fig. 6** [34]. The density of states spectra were created by convoluting the molecular orbital information with the Gaussian curves of unit height[35,36]. The green and blue lines in the density of states spectrum indicate the Highest Occupied Molecular Orbitals and Lowest Unoccupied Molecular Orbitals levels respectively.



**Fig. 5** HOMO and LUMO plots of 2-(4-Isobutylphenyl) propanoic acid



**Fig. 6** DOS spectrum of 2-(4-Isobutylphenyl) propanoic acid

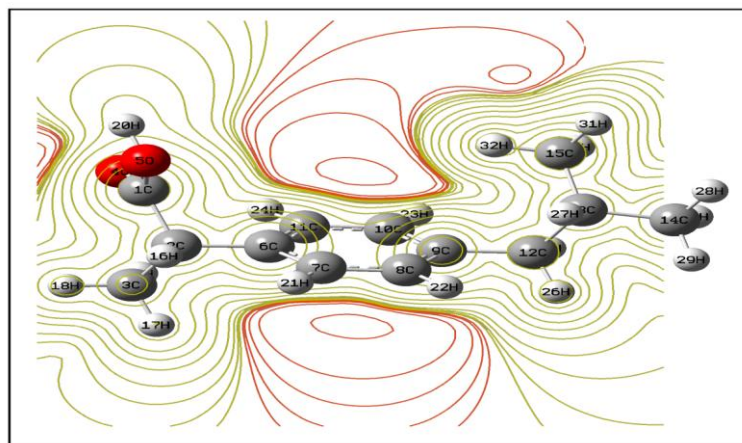
**Table 7 HOMO-LUMO energy gap and physico-chemical properties of 2-(4-Isobutylphenyl) propanoic acid**

Parameters (eV)	B3LYP/6-311++G(d, p)
HOMO Energy	6.6856
LUMO Energy	0.8019
HOMO - LUMO Energy	5.8837
Ionization potential (I)	-6.6856
Electrophilicity ( $\omega$ )	-2.3820
Electro negativity ( $\chi$ )	-3.7437
Electron affinity (A)	-0.8019
Global hardness ( $\eta$ )	-2.9418
Global softness (S)	-0.3399
Chemical potential ( $\mu$ )	3.7437

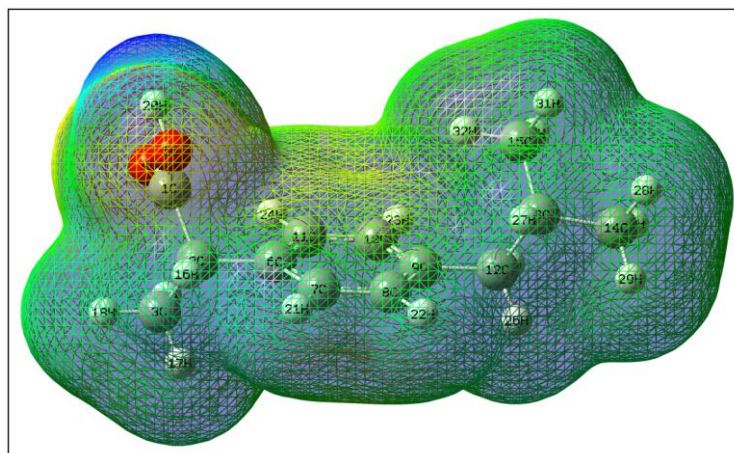
#### 4.8 MESP Analysis

The MESP surfaces have been plotted for 2-(4-Isobutylphenyl)propanoic acid in B3LYP/6-311++G (d,p) method using the computer software GaussView 5.0. The molecular electrostatic potential contour surface of 2-(4-Isobutylphenyl)propanoic acid is presented in the **Fig. 7**. The molecular electrostatic potential surface of 2-(4-Isobutylphenyl)propanoic acid is presented in the **Fig. 8**. The molecular electrostatic potential correlates with electro negativity, dipole moment, partial charges and site of chemical reactivity of the molecule. Such surfaces depict the shape, size, charge density and site of chemical reactivity. It provides a visual method to understand the relative polarity of the molecule. The potential increases in the order red colour < yellow colour < green colour < light blue colour < blue colour where red colour indicates the lowest molecular electrostatic potential energy and blue colour indicates the highest molecular electrostatic potential energy [37]. The intermediary colours represent intermediary molecular electrostatic potentials. The colour scheme for the molecular electrostatic potentials surface is red colour-electron rich, partially negative charge; yellow colour-slightly electron rich region; green colour-neutral; light blue colour-slightly electron deficient region and blue colour-electron deficient, partially positive charge. The MESP surface shows the positive potential sites are on hydrogen atoms as well as the negative potential sites are around the oxygen atoms [38, 39]. The H atoms indicate the strongest attraction and O atoms indicated the strongest repulsion of the electron density [40]. In the case of 2-(4-Isobutylphenyl)propanoic acid molecule the negative regions are mainly localized on the

oxygen (O<sub>4</sub> and O<sub>5</sub>) atoms. The oxygen atoms have a higher electro negativity value; it would consequently have a higher electron density plot for the molecule. Thus the spherical region that corresponds to oxygen atom would have a red colour portion on it.



**Fig. 7** MESP contour surface of 2-(4-Isobutylphenyl) propanoic acid



**Fig. 8** MESP of 2-(4-Isobutylphenyl) propanoic acid

## 4.9 Conclusion

The density functional theory calculated geometrical parameters were found to be in good agreement with the observed data. A complete vibrational analysis of 2-(4-Isobutylphenyl) propanoic acid is performed by B3LYP with 6-311++G (d,p) basis set. The observed and computed wavenumbers are found to be in good agreement with the observed FT-IR spectral values. The intramolecular interactions and stability have been interpreted by natural bond analysis and the transactions give stabilization to the structure have been identified by the second perturbation energy calculations. The natural atomic charges of the title molecule have been studied by the NBO analysis. Thermodynamic properties such as zero-point vibrational energies, thermal energy, molar capacity at constant volume, rotational constant, entropy and dipole moment are also calculated. The absorption maxima ( $\lambda_{\text{max}}$ ) of 2-(4-Isobutylphenyl) propanoic acid was calculated by the TD-DFT/B3LYP with 6-311++G (d,p) method and compared with the observed UV-Visible spectrum. The Highest Occupied Molecular Orbitals and Lowest Unoccupied Molecular Orbitals have been visualized. The computed HOMO and LUMO energies can be used to estimate the electro negativity, ionization potential, global hardness, electron affinity, electrophilicity, global softness and chemical potential. The MESP map shows the negative potential sites are on O atoms as well as the positive potential sites are around the H atoms.

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