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Theoritical Investigations on Molecular Structure Vibrational Spectra, Mulliken Atomic Charge and HOMO-LUMO, Analysis of O-(Salicyloyloxy) Benzoic Acid

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ABSTRACT

The experimental FT-IR (4000 - 400 cm-1) and FT- Raman (3500 - 100 cm-1) spectra of o-(salicyloyloxy) benzoiacid (OSBA) have been recorded. Quantum chemical calculation of energies, geometric, vibrational wave numbers of OSBA are carrier out using DFT/B3LYP method 6-31+G (d) and 6-311++G (d, p) basic sets. The optimized geometrical parameters obtained by B3LYP method shows a good agreement with experimental data. The complete vibrational assignments were performed on the basics of potential energy distribution (PED) of the vibrational modes calculated with scaled quantum mechanical method. The calculated HOMO and LUMO energies allow the calculation of atomic and molecular properties and they also show that charge transfer occurs in the molecule. Details of molecular picture of OSBA, Mulliken atomic charge and molecular electrostatic potential map, respectively.

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1. INTRODUCTION

The sample name of O-(salicyloyloxy) benzoic acid is salsalate. It is a non-steroidal ant-inflammatory drug used for decades to relive pain, tenderness, swelling, and stiffness caused by rheumatoid arthritis has now been shown to reduce blood glucose leaves in individuals with type 2-diabetes. It has also been used as an alternative to narcotic pain medicine for people with spinal disc protrusion. The molecular formula for o-(salicyloyloxy) benzoic acid is $C_{14}H_{10}O_5$. It is a white crystalline powder and soluble in organic solvents such as ethanol, DMSO and acetone. The hydrogen bonding in salicylosalicylic acid crystal was described in literature [1]. The Fluorimetric determination of salsalate in urine, serum and Pharmaceutical preparations were reported by Pulgarin and Bermejo [2]. The simultaneous TG-DTA study of the thermal decomposition of o-(salicyloyloxy) benzoic acid ester has been studied [3]. Hemostatic effects of salsalate were and changes in thyroid function tests during short-term salsalate were reported earlier [4, 5].

Inspire of its importance for Pharmaceutical purpose, the reported spectroscopic studies on OSPA are scarce. The evolution of density function theory that includes electron correlation in an alternative way has affording opportunities of performing vibrational analysis of moderately large organic molecular. The results for DFT theory with results obtained from experiments has shown that the methods using B3LYP are the most promising in providing correct vibrational wave numbers. The kinetics and decomposing o-(salicyloyloxy) benzoic acid have been studied with the help of thermo gravimetric-differential thermal analysis (TG-DTA) and gas and liquid chromatography [6]. The hydrogen bonding in the salsalate crystal was previously carried out and

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the position of hydroxyl group in ortho position on an aryl ring with possible intermolecular hydrogen bonds are discussed with the crystal data collected at low temperature [7]. From the crystal data, the structure of the molecule was determined and there's no information about the structure conformation and vibrational analysis of the molecule. Literature survey reveals that so far there is no complete theoretical study for the title compound OSBA. In this study, we sat out experimental and theoretical investigation of the conformation, vibration and electron transition of OSBA. In the ground state theoretical geometrical parameters, IR, Raman and HOMO and LUMO energies of title molecule were calculated by using Gaussian 09 programming. Detailed interpretations of the vibrational spectra of the basis of the calculate potential energy distribution (PED). The experimental results (IR, Raman) were supported by the computed results. comparing with experimental characterization data, vibrational wave numbers and absorption wave length values are in fairly good agreement with the experimental results. The stable position with respect to pyridine ring was obtained by performing the potential energy surface (PES) scans with B3LYP/6-31+G (d) and B3LYP/6-311++G (d, p) level of theory. By analyzing the total density of state (TDOS) and partial density of state (PDOS), the molecular orbital compositions and their contributions to the chemical bonding were studied. The study of the HOMO and LUMO analysis has been used to elucidate information recording charge transfer within the molecule. Moreover, the Mulliken population analyses of the title compound have been reported. The experimental and theoretical results supported each other, and the calculations

are valuable for providing a reliable inside in to the vibrational spectra and molecules properties.

2. EXPERIMENTAL DETAILS

The sample O-(salicyloyloxy) benzoic acid from was purchased from the Sigma-Aldrich chemical company (USA) with a stated purity of greater than 98% and it was used as such without further purification. The FT-IR spectrum of molecule was recorded in the region 4000-400 cm⁻¹. The FT-Raman spectrum of OSPA title molecule has been recorded in the region from wavelength is 3500-100 cm⁻¹.

3. COMPUTATIONAL Details

The entire calculation ware performed at DFT/B3LYP with the standard basis set 6-31+G (d) and 6-31++G (d, p) on personal computer using GAUSSIAN 09W program package. invoking gradient geometry optimization [8]. The optimized structure used in the vibrational wave number calculation at the B3LYP with using 6-31+G (d) and 6-31++G (d, p) levels. Subsequently, the vibrational association with the molecule was derived along with their IR intensity and Raman activity. In order to fit the theoretical wave numbers to the experimental, the scaling factors have been introduced by using a least square optimization method. The polarizability, first hyperpolarizability and dipole moments of OSPA have been calculated using the same method. The HOMO-LUMO analysis has been carried out to explain the charge transfer within the molecule. Have been calculated using the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO). To check whether the chosen set of symmetric coordinates contributes maximum to the potential energy associated with the molecule, the PED has been carries out. The total density of state (TDOS), the partially density of states (PDOS) are prepared by using the programming Gauss sum 2.2 [9] and the functional group contribution to the molecular orbital's are calculated.

4. RESULT AND DISCUSSION 4.1. STRUCTURAL PROPERTIES

The optimized geometry structural parameters bond length and bond angle for the thermodynamically performed of OSBA are determine at B3LYP level with 6-31+G (d) and 6-311++G (d, p) basis set and visualized using GAUSSIAN and GAUSSVIEW program is shown in Fig 1. The molecule consist of 29 atoms and expected to have 81 normal modes of fundamental vibration out of which 28 modes are stretching type and 53 are of bending type. This molecule has four C-O bond length, two C-C, C=O and O-H bond length and eight C-H bond length. The C-H bond length in the optimized geometry of OSBA calculated at both levels fall in the range; 1.09-1.11A°. It is close agreement with the experimental values [10].



Fig. 1. The theoretical geometry structure and atomic numbering scheme of O-(Salicyloyloxy) benzoicacid.

The optimized bond length, bond angles and Dihedral angle of the title was compound which are calculated using B3LYP method 6-31+G (d) and 6-311++G (d, p) basis sets

are given in Table 1. The optimized geometrical parameter of the title compound was compared with other similar system for which the crystal structure has been solved [11].

4.2 VIBRATIONAL ASSIGNMENTS

The virational band assignments to the observed bands of OSBA have been made in accordance with the position, shape, nature and relative intensities of the recorded spectra. The assignments have been made in analog with the structurally related molecules. On the basis of theoretical investigation as discussed earlier, the atoms of the compound have 29 atoms and the three Cartesian displacements of the compound provide 81 internal modes out of which 28 vibration (stretching). The assignments of the experimental wave numbers based on normal mode analyses are provide in Table 2. In general, DFT calculations systematically overestimate the vibrational wave numbers. The frequency observed in FT-IR spectrum at 815 cm⁻¹ have been assigned to ring breathing and corresponding vibration appear in FT-Raman spectrum at 812 cm⁻¹ shows good agreement with experimental values. Usually an in-plane deformation is at higher frequencies than the out-of-plane deformations [12]. The observed FT-IR and FT-Raman spectra of OSBA along with the simulated infrared and Raman spectra are shown in Figs. 2 and 3.



Fig 2. Comparative representation of FT-IR spectra for O-(Salicyloyloxy) benzoicacid.

Ring vibration

The position and intensity of ring stretching vibration depend on the nature of the ring and the type of substitution. The aromatic ring vibrational modes of title molecule have been analyzed based on the vibrational spectra of previously published vibration of benzene molecule is more helpful in the identification of the phenyl ring modes. The ring stretching



Fig. 3. Comparative representation of FT-Raman spectra for O-(Salicyloyloxy)benzoicacid.

T. Rajalakshmy et al./ Elixir Computational physics 116 (2018) 50292-50301 Table 1.Optimized geometrical parameters of O-(Salicyloyloxy) benzoic acid by B3LYP/6-31+G (d) and B3LYP/6-311++G (d, p) methods.

	Bo	ond length (Å))		Bond angle (degrees)			Dihedra (deg	ll angles rees)	
Parameters	B3L	YP		Parameters	B3L	YP		Parameters	B3I	.YP
	6-31+G(d)	6-311++ G(d,p)	Exp.*		6-31+G(d)	6-311++ G(d,p)	Exp.*		6-31+G(d)	6-311++G (d, p)
C ₁ -C ₂	1.408	1.405	1.3979	$C_2 - C_1 - C_6$	120.68	120.59	-	$C_6-C_1-C_2-C_3$	0.55	0.61
C_1-C_6	1.394	1.391	1.3816	$C_2 - C_1 - O_{15}$	122.64	122.98	-	$C_6 - C_1 - C_2 - C_7$	-179.49	-179.40
C ₁ -O ₁₅	1.389	1.387		$C_6 - C_1 - O_{15}$	116.59	116.36	-	$O_{15}-C_1-C_2-C_3$	176.93	177.41
C ₂ -C ₃	1.407	1.403	1.3987	$C_1 - C_2 - C_3$	118.05	118.05	-	$O_{15}-C_1-C_2-C_7$	-3.10	-2.60
C ₂ -C ₇	1.491	1.491	1.4722	$C_1 - C_2 - C_7$	126.01	126.14	119.95	$C_2 - C_1 - C_6 - C_5$	-0.22	-0.08
C ₃ -C ₄	1.391	1.387	1.3851	$C_3-C_2-C_7$	115.94	115.81	121.05	C ₂ -C ₁ -C ₆ -H ₁₄	179.94	-179.99
C ₃ -H ₁₁	1.085	1.083	-	$C_2-C_3-C_4$	121.46	121.50	121.05	$O_{15}-C_1-C_6-C_5$	-176.81	-177.08
C ₄ -C ₅	1.398	1.394	1.3990	C ₂ -C ₃ -H ₁₁	117.63	117.56	-	O ₁₅ -C ₁ -C ₆ -H ₁₄	3.35	3.01
C ₄ -H ₁₂	1.086	1.083	-	C ₄ -C ₃ -H ₁₁	120.91	120.94	-	$C_2 - C_1 - O_{15} - C_{16}$	81.58	77.66
C_5-C_6	1.394	1.390	1.4032	$C_3-C_4-C_5$	119.59	119.56	119.60	$C_6 - C_1 - O_{15} - C_{16}$	-101.90	-105.42
C ₅ -H ₁₃	1.087	1.084	1.3497	C ₃ -C ₄ -H ₁₂	119.97	120.01	123.24	$C_1 - C_2 - C_3 - C_4$	-0.52	-0.72
C ₆ -H ₁₄	1.086	1.083	-	C ₅ -C ₄ -H ₁₂	120.44	120.43	-	C ₁ -C ₂ -C ₃ -H ₁₁	179.58	179.42
C ₇ -O ₈	1.218	1.209	1.2619	$C_4-C_5-C_6$	119.94	119.96	-	$C_7 - C_2 - C_3 - C_4$	179.52	179.29
C ₇ -O ₉	1.356	1.354	1.2904	C ₄ -C ₅ -H ₁₃	120.39	120.38	-	C ₇ -C ₂ -C ₃ -H ₁₁	-0.38	-0.58
O ₉ -H ₁₀	0.976	0.969	-	C ₆ -C ₅ -H ₁₃	119.67	119.66	-	$C_1 - C_2 - C_7 - O_8$	-175.72	-172.58
H ₁₄ -O ₁₇	3.642	3.718	-	$C_1 - C_6 - C_5$	120.H28	120.34	-	$C_1 - C_2 - C_7 - O_9$	5.09	8.51
O ₁₅ -C ₁₆	1.386	1.385	-	C ₁ -C ₆ -H ₁₄	118.42	118.36	-	$C_3 - C_2 - C_7 - O_8$	4.25	7.41
C ₁₆ -O ₁₇	1.207	1.199	-	C ₅ -C ₆ -H ₁₄	121.30	121.30	122.92	C ₃ -C ₂ -C ₇ -O ₉	-174.95	-171.50
C ₁₆ -C ₁₈	1.485	1.485	-	C ₂ -C ₇ -O ₈	123.73	123.78	-	$C_2 - C_3 - C_4 - C_5$	0.15	0.29
C ₁₈ -C ₁₉	1.414	1.411	-	$C_2 - C_7 - O_9$	115.00	114.71	-	$C_2-C_3-C_4-H_{12}$	-179.85	-179.73
C ₁₈ -C ₂₃	1.407	1.403	-	O ₈ -C ₇ -O ₉	121.26	121.50	-	$H_{11}-C_3-C_4-C_5$	-179.96	-179.85
C ₁₉ -C ₂₀	1.403	1.400	1.3336	C ₇ -O ₉ -H ₁₀	105.92	106.18	-	H ₁₁ -C ₃ -C ₄ -H ₁₂	0.05	0.13
C ₁₉ -O ₂₄	1.359	1.356	1.3429	$C_1 - O_{15} - C_{16}$	118.06	118.35	-	$C_3 - C_4 - C_5 - C_6$	0.20	0.26
C ₂₀ -C ₂₁	1.392	1.389	1.3354	O ₁₅ -C ₁₆ -O ₁₇	122.23	122.38	-	C ₃ -C ₄ -C ₅ -H ₁₃	179.95	179.94
C ₂₀ -H ₂₆	1.089	1.086	-	$O_{15}-C_{16}-C_{18}$	110.57	110.29	-	$H_{12}-C_4-C_5-C_6$	-179.81	-179.72
C ₂₁ -C ₂₂	1.399	1.395	1.3358	$O_{17}-C_{16}-C_{18}$	127.20	127.33	-	$H_{12}-C_4-C_5-H_{13}$	-0.05	-0.04
C ₂₁ -H ₂₇	1.087	1.084	-	C ₁₆ -C1 ₈ -C ₁₉	121.07	121.03	-	$C_4 - C_5 - C_6 - C_1$	-0.16	-0.37
C ₂₂ -C ₂₃	1.392	1.388	1.3497	$C_{16}-C_{18}-C_{23}$	120.41	120.34	-	C ₄ -C ₅ -C ₆ -H ₁₄	179.67	179.54
C ₂₂ -H ₂₈	1.086	1.083	-	$C_{19}-C_{18}-C_{23}$	118.50	118.61	-	$H_{13}-C_5-C_6-C_1$	-179.92	179.96
C ₂₃ -H ₂₉	1.084	1.081	-	$C_{18}-C_{19}-C_{20}$	119.64	119.57	-	H ₁₃ -C ₅ -C ₆ -H ₁₄	-0.09	-0.13
O ₂₄ -H ₂₅	0.971	0.964	1.4406	$C_{18}-C_{19}-O_{24}$	119.36	119.37	-	C ₂ -C ₇ -O ₉ -H ₁₀	-179.03	-178.69
				$C_{20}-C_{19}-O_{24}$	120.99	121.06	118.77	O ₈ -C ₇ -O ₉ -H ₁₀	1.75	2.37
				$C_{19}-C_{20}-C_{21}$	120.72	120.72	115.10	$C_1 - O_{15} - C_{16} - O_{17}$	4.12	4.19
				C ₁₉ -C ₂₀ -H ₂₆	119.12	119.10	-	$C_1 - O_{15} - C_{16} - C_{18}$	-176.29	-176.01
				C ₂₁ -C ₂₀ -H ₂₆	120.16	120.18	-	O_{15} - C_{16} - C_{18} - C_{19}	-162.48	-158.80
				$C_{20}-C_{21}-C_{22}$	120.23	120.25	127.30	$O_{15}-C_{16}-C_{18}-C_{23}$	18.74	22.85
				C ₂₀ -C ₂₁ -H ₂₇	119.41	119.43	-	O_{17} - C_{16} - C_{18} - C_{19}	17.08	20.99
				C ₂₂ -C ₂₁ -H ₂₇	120.36	120.32	-	$O_{17}-C_{16}-C_{18}-C_{23}$	-161.70	-157.36
				C_{21} - C_{22} - C_{23}	119.24	119.25	115.43	$C_{16} - C_{18} - C_{19} - C_{20}$	-178.72	-178.13
				C ₂₁ -C ₂₂ -H ₂₈	120.57	120.53	-	$C_{16} - C_{18} - C_{19} - O_{24}$	2.32	3.13
				C ₂₃ -C ₂₂ -H ₂₈	120.19	120.22	-	C_{23} - C_{18} - C_{19} - C_{20}	0.08	0.25

T. R	ajalakshmy	et al./ Elixir Comp	utational phy	vsics 116 (20	18) 50292-5	50301	
		C_{18} - C_{23} - C_{22}	121.67	121.60	-	C ₂₃ -C ₁₈ -C ₁₉ -O ₂₄	
			110.15	110.10		0 0 0 0	1

		C_{18} - C_{23} - C_{22}	121.67	121.60	-	C_{23} - C_{18} - C_{19} - O_{24}	-178.88	-178.49
		C ₁₈ -C ₂₃ -H ₂₉	118.15	118.10	-	C_{16} - C_{18} - C_{23} - C_{22}	178.37	177.70
		C ₂₂ -C ₂₃ -H ₂₉	120.17	120.30	116.61	C ₁₆ -C ₁₈ -C ₂₃ -H ₂₉	-1.01	-1.59
		C ₁₉ -O ₂₄ -H ₂₅	109.36	109.38	-	C_{19} - C_{18} - C_{23} - C_{22}	-0.45	-0.69
						C ₁₉ -C ₁₈ -C ₂₃ -H ₂₉	-179.82	-179.98
						$C_{18}-C_{19}-C_{20}-C_{21}$	0.31	0.33
						C ₁₈ -C ₁₉ -C ₂₀ -H ₂₆	-179.67	-179.64
						$O_{24}-C_{19}-C_{20}-C_{21}$	179.25	179.05
						O ₂₄ -C ₁₉ -C ₂₀ -H ₂₆	-0.73	-0.92
						C ₁₈ -C ₁₉ -O ₂₄ -H ₂₅	178.15	178.62
						C ₂₀ -C ₁₉ -O ₂₄ -H ₂₅	-0.79	-0.10
						C_{19} - C_{20} - C_{21} - C_{22}	-0.35	-0.49
						C ₁₉ -C ₂₀ -C ₂₁ -H ₂₇	179.76	179.72
						$H_{26}-C_{20}-C_{21}-C_{22}$	179.63	179.48
						H ₂₆ -C ₂₀ -C ₂₁ -H ₂₇	-0.25	-0.31
						$C_{20}-C_{21}-C_{22}-C_{23}$	-0.01	0.06
						C ₂₀ -C ₂₁ -C ₂₂ -H ₂₈	179.95	-179.98
						$H_{27}-C_{21}-C_{22}-C_{23}$	179.87	179.84
						H_{27} - C_{21} - C_{22} - H_{28}	-0.17	-0.20
						C_{21} - C_{22} - C_{23} - C_{18}	0.41	0.54
						C ₂₁ -C ₂₂ -C ₂₃ -H ₂₉	179.77	179.81
						$H_{28}-C_{22}-C_{23}-C_{18}$	-179.54	-179.42
						H ₂₈ -C ₂₂ -C ₂₃ -H ₂₉	-0.18	-0.15

Notes: Bond length is in Å, bond angle and dihedral angle are in degrees

Table 2. Vibrational assignments of FT-IR and FT-Raman peaks along theoretically computed wave numbers, IR intensity (I _{IR}) and Raman intensity (I _{Raman}) and the	he
percentage of potential distribution of O-(Salicyloyloxy) benzoic acid.	

		Observed wave number(cm ⁻¹)		B3LYP/6-31+G (d)					B3LYP/6-31		- Assignments with %	
Sl. No	Species	FT-IR	FT- Raman	Calculated wave number(cm ⁻¹)		I _{IR}	I _{Raman}	Calculat numbe	ted wave r(cm ⁻¹)	1 wave cm ⁻¹) I _{IR}		of PED ^c
		Kaman		Un scaled	Scaled			Un scaled	Scaled			
1	А			3743	3498	53.630	163.886	3824	3492	72.068	149.253	υOH(100)
2	А	3466		3689	3468	73.482	106.698	3761	3463	86.244	102.125	υOH(100)
3	А			3241	3102	2.027	94.360	3219	3098	1.674	99.408	υCH(56)
4	А			3230	3087	4.935	155.534	3207	3086	5.367	188.293	υCH(62)
5	А		3071	3219	3073	6.246	137.234	3200	3070	3.149	103.686	υCH(74)
6	А			3211	3064	16.792	200.698	3193	3061	11.441	186.790	υCH(91)
7	А			3208	3059	16.320	143.369	3189	3053	10.925	132.113	υCH(74)
8	А	2933		3195	3044	9.922	118.335	3176	3041	7.401	115.752	υCH(64)
9	А			3193	3040	3.376	74.047	3174	3038	2.739	68.112	υCH(65)
10	А	2866		3167	2870	14.283	109.053	3150	2867	11.173	103.742	υCH(93)
11	Α	1744		1812	1747	304.012	115.947	1809	1742	317.507	113.547	υC=O(87)
12	А	1678	1672	1782	1678	417.927	71.223	1777	1673	419.895	67.040	υC=O(83)

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T. Rajalakshmy et al./ Elixir Computational physics 116 (2018) 50292-50301

13	А		1627	1657	1629	31.969	57.566	1646	1624	32.371	53.042	υCC(64), βCH(9)
14	А	1611		1655	1613	102.268	95.005	1644	1611	101.052	94.639	υCC(60), βCH(17)
15	А		1593	1637	1596	38.447	27.488	1626	1590	36.463	23.585	υCC(48), βCH(18)
16	А	1577		1623	1579	7.474	10.946	1612	1574	7.540	10.685	υCC(54), βCH(21)
17	А	1466		1541	1468	17.545	13.440	1529	1465	18.526	12.702	υCC(61), βCH(26)
18	А		1453	1524	1457	29.224	3.522	1511	1453	29.070	3.282	υCC(57), βCH(17)
19	А	1411		1492	1416	81.224	0.771	1481	1410	77.548	0.681	υCC(61), βCH(16)
20	А	1376	1377	1490	1375	56.894	4.801	1479	1371	59.003	4.144	υCC(68)
21	А			1384	1342	139.093	10.174	1372	1340	127.495	9.503	υCC(63), βCH(12)
22	А	1333		1378	1337	31.942	5.497	1362	1334	37.803	4.683	υCC(62)
23	А		1325	1353	1327	13.423	7.804	1336	1326	21.283	5.901	υC-O(64)
24	А	1300	1302	1343	1304	80.362	13.502	1332	1298	60.936	14.011	υC-O(71)
25	А	1277		1302	1280	19.814	3.518	1292	1276	9.108	2.340	υC-O(73)
26	А		1255	1297	1258	41.429	0.564	1289	1254	52.717	2.100	υC-O(68)
27	А	1244		1265	1246	273.022	54.288	1256	1245	231.661	50.487	υCC(54), βCH(16)
28	А		1209	1229	1210	602.876	78.202	1218	1208	558.067	41.736	υCC(51), CH(21)
29	А	1199		1216	1200	64.933	73.967	1207	1198	72.903	98.915	βCH(46)
30	А			1204	1186	29.670	5.473	1196	1183	29.523	4.793	υCH(51)
31	А	1166		1184	1167	35.085	10.251	1185	1165	40.229	11.271	βOH(48)
32	А		1151	1171	1152	15.726	22.679	1180	1150	23.167	28.907	βOH(54)
33	А	1133		1145	1136	204.037	1.497	1137	1134	214.721	1.980	CH(51)
34	А			1134	1127	46.209	2.637	1126	1125	64.012	1.812	βCH(48)
35	A	1099		1110	1101	13.648	3.413	1103	1100	11.163	4.634	βCH(51)
36	A	1063	1062	1073	1064	7.545	49.352	1067	1064	4.557	48.839	βCH(46)
37	A	1000	1034	1065	1035	67.850	24.001	1059	1033	79.704	27.038	βCH(63)
38	A	1022	0.65	1040	1023	267.612	8.592	1029	1022	327.832	10.386	βCH(57)
39	A	055	965	1005	967	0.330	0.112	1003	965	0.433	0.048	$\upsilon CC(47)$
40	A	955		991	956	0.092	0.092	990	954	0.270	0.029	UCC(42)
41	A	933	007	982	934	1.890	0.119	984	932	1.958	0.076	υCC(66)
42	A	000	906	936	907	0.682	0.116	935	905	0.771	0.086	UCC(54)
43	A	888		919	890	7.230	1.935	918	887	9.416	1.945	υCC(51)
44	A	866	0.40	875	868	13.377	5.349	874	864	15.543	5.429	γCH(53)
45	A	020	848	862	849	5.884	0.510	860	846	8.655	1.015	γCH(42)
46	A	829	828	849	830	20.700	8.163	848	827	17.949	7.288	γCH(43)
4/	A	811	700	828	813	2.570	17.443	827	810	3.904	15.422	βC-O(46)
48	A	777	/98	808	799	0.293	0.418	810	797	0.441	0.445	pC-0(51)
49	A	777	779	/80	778	4.505	1.964	/88	7754	2.939	2.800	$\gamma CH(41)$
50	A	/55	/56	/65	757	69.649 51.416	2.001	/63	754	/1.124	1.445	γCH (42)
51	A	700		/58	742	51.416	2.297	/58	741	45.969	2.765	$\gamma CH(47)$
52	A	122	(00	/50	/20	23.123	15.159	/49	/21	20.354	15./6/	γCH(40)
55	A	689	690	/14	690	57.289	8.680	/15	689	3/.43/	8.059	γCH(48)
54	A	640	649	692	6/0	10.091	0.491	699 275	008 249	10.81/	0.772	BCCC(41)
56	A A	049	048 607	626	607	20.393	4.382	639	605	21.032	4.337	$\beta CCC(47)$
57	A	580	007	618	5007	29.301 18.087	2.200	607	580	11 /32	2.377	BCCC(49)
57	А	509		010	390	40.90/	1.940	007	209	11.433	∠.900	pccc(32)

50297

T. Rajalakshmy et al./ Elixir Computational physics 116 (2018) 50292-50301

58A604576 4.393 2.391 602573 45.081 1.513 $\gamma CH(50)$ 59A564572565 2.718 8.568 573564 3.203 8.591 $\gamma CH(49)$ 60A544558543 4.992 1.419 559541 3.860 1.384 $\gamma CH(54)$ 61A522523538524 7.325 0.473 536523 5.208 0.566 $\gamma CH(57), \gamma CH(14)$ 62A-522513 2.280 1.850 520 512 2.068 1.748 $\beta CCC(56),$ 63A4477489478 14.578 5.626 488476 13.665 5.912 $\beta CCC(46), \gamma CH(17),$ 64A441449443 5.371 0.187 447441 2.706 0.215 $\gamma C·O(43)$ 65A408419407 5.983 0.241 416406 7.843 0.298 $\gamma C·O(42)$ 66A-407391 52.349 2.237 402390 6.308 1.576 $\gamma C·O(42)$ 67A-377330315 0.732 2.212 329316 8.986 1.660 $\gamma OH(46)$ 70A294308297 2.872 0.595 306294 2.949 0.606 $\gamma OH(51)$ 71A271292273 0.484 1.726 <th></th> <th></th> <th></th> <th></th> <th></th> <th></th> <th></th> <th></th> <th></th> <th>,</th> <th>-</th> <th></th> <th></th>										,	-		
59 A 564 572 565 2.718 8.568 573 564 3.203 8.591 YCH(49) 60 A 544 558 543 4.992 1.1419 559 541 3.860 1.384 YCH(54) 61 A 522 523 538 524 7.325 0.473 536 523 5.208 0.566 YCH(54) 62 A - 522 513 2.280 1.850 520 512 2.068 1.748 BCCC(56), 63 A - 441 449 443 5.371 0.187 447 441 2.706 0.215 yC-0(43) 64 A - 407 391 52.349 2.237 402 390 6.308 1.576 yC-0(43) 65 A - 374 390 373 4.639 3.66 362 369 3.958 2.327 yCC(40) 67<	58	А			604	576	4.393	2.391	602	573	45.081	1.513	γCH(50)
60A5445585434.9921.4195595413.8601.384 γ CH(54)61A5225235385247.3250.4735365235.2080.566 γ CH(57), γ CH(14)62A5225132.2801.8505205122.0681.748 β CC(56),63A4774494435.710.1874474412.7060.215 γ C-0(46), γ CH(17)64A4414494435.3710.1874474412.7060.215 γ C-0(46)65A4084194075.9830.2414164067.8430.298 γ C-0(42)66A40739152.3492.2374023906.3081.576 γ C-0(42)67A3743903734.6393.0663623693.9582.327 γ CC(40)68A3173303150.7322.21232931686.9861.660 γ OH(5)70A2943082972.8720.5953062942.9490.606 γ OH(5)71A2712922730.8421.7262712712.2891.841 γ C=0(4)71A2712922730.8421.7262712712.2891.841 γ C=0(4)72A1681680.	59	А		564	572	565	2.718	8.568	573	564	3.203	8.591	γCH(49)
61A522523538524 7.325 0.473 536523 5.208 0.566 $\gamma CH(57), \gamma CH(14)$ 62A-522513 2.280 1.850 520 512 2.068 1.748 $\beta CCC(56),$ 63A477489478 14.578 5.626 488 476 13.665 5.912 $\beta CCO(46), \gamma CH(17)$ 64A441449443 5.371 0.187 447 441 2.706 0.215 $\gamma C-O(46), \gamma CH(27)$ 65A408419407 5.983 0.241 416406 7.843 0.298 $\gamma C-O(43)$ 66A-407391 52.349 2.237 402390 6.308 1.576 $\gamma C-O(42)$ 67A-397 382 49.349 1.447 389 380 4.868 2.464 $\gamma C-O(43)$ 68A-374390373 4.639 3.066 362 369 3.958 2.327 $\gamma CCC(40)$ 69A317330315 0.732 2.212 329 316 86.96 1.660 $\gamma OH(46)$ 70A294 308 297 2.872 0.595 306 2.949 0.606 $\gamma OH(51)$ 71A237245237 1.146 0.884 243236 0.891 0.638 $\gamma C-O(42)$ 71A179199180 <td>60</td> <td>А</td> <td>544</td> <td></td> <td>558</td> <td>543</td> <td>4.992</td> <td>1.419</td> <td>559</td> <td>541</td> <td>3.860</td> <td>1.384</td> <td>γCH(54)</td>	60	А	544		558	543	4.992	1.419	559	541	3.860	1.384	γCH(54)
62A5225132.2801.8505205122.0681.748 β CCC(56),63A47748947814.5785.62648847613.6655.912 β CCC(46), γ CH(17)64A4414494435.3710.1874474412.7060.215 γ CO(46)65A4084194075.9830.2414164067.8430.298 γ C-O(42)66A40739152.3492.2374023906.3081.576 γ C-O(42)67A39738249.3491.4473893804.8682.464 γ C-O(43)68A3743903734.6393.0663623693.9582.327 γ CCC(40)69A3173303150.7322.21232931686.9861.660 γ OH(46)71A2712922730.8421.7262712712.2891.841 γ C=O(41)72A2372452371.1460.8842432360.8910.638 γ C=O(42)73A1791991802.4400.4201971782.4660.431 γ CCC(37)74A1681860.6431.4401861670.4001.285 γ CCC(40)76A1211060.4722.135118<	61	А	522	523	538	524	7.325	0.473	536	523	5.208	0.566	γCH(57), γCH(14)
63A47748947814.5785.62648847613.6655.912 β CCC(46), γ CH(17)64A4414494435.3710.1874474412.7060.215 γ C-0(46)65A4084194075.9830.2414164067.8430.298 γ C-0(43)66A40739152.3492.2374023906.3081.576 γ C-0(42)67A40739738249.3491.4473893804.8682.464 γ C-0(43)68A3743903734.6393.0663623693.9582.327 γ CC(40)69A3173303150.7322.21232931686.9861.660 γ OH(46)70A2943082972.8720.5953062942.9490.606 γ OH(51)71A2712922730.8421.7262712712.2891.841 γ C-0(41)72A2372452371.1460.8842432360.8910.638 γ C-0(42)73A1791991802.4400.4201971782.4660.431 γ CCC(40)74A1681861680.4541.4401861670.4001.285 γ CCC(40)75A1301160.5	62	А			522	513	2.280	1.850	520	512	2.068	1.748	βCCC(56),
64 A 441 449 443 5.371 0.187 447 441 2.706 0.215 γ C-0(46) 65 A 408 419 407 5.983 0.241 416 406 7.843 0.298 γ C-0(42) 66 A 407 391 52.983 0.241 416 406 7.843 0.298 γ C-0(42) 67 A 407 391 52.37 402 390 6.308 1.576 γ C-0(42) 67 A 397 382 49.349 1.447 389 380 4.868 2.464 γ C-0(43) 68 A 374 390 373 4.639 3.066 362 369 3.588 2.327 γ CC(40) 69 A 317 330 315 0.732 2.212 329 316 86.986 1.660 γ OH(46) 70 A 294 308 297 2.872 0.595 306 294 2.949 0.606 γ OH(51) 71 A 271 292 273 0.842 1.726 271 2.189 1.841 γ C=0(41) 72 A 237 245 237 1.146 0.884 243 236 0.891 0.638 γ C=0(42) 73 A 179 199 180 2.440 1400 186 167 0.400 1.285 γ CCC(45) 75 A 163 166 0.472	63	А		477	489	478	14.578	5.626	488	476	13.665	5.912	βCCC(46), γCH(17)
65 A 408 419 407 5.983 0.241 416 406 7.843 0.298 γ C- $0(43)$ 66 A 407 391 52.349 2.237 402 390 6.308 1.576 γ C- $0(42)$ 67 A 397 382 49.349 1.447 389 380 4.868 2.464 γ C- $0(43)$ 68 A 374 390 373 4.639 3.066 362 369 3.958 2.327 γ CC(40) 69 A 317 330 315 0.732 2.212 329 316 86.986 1.660 γ OH(46) 70 A 294 308 297 2.872 0.595 306 294 2.949 0.606 γ OH(46) 71 A 271 292 273 0.842 1.726 2711 2.189 1.841 γ C= $0(41)$ 72 A 237 245 237 1.146 0.884 243 236 0.891 0.638 γ C= $0(42)$ 73 A 179 199 180 2.440 0.420 197 178 2.466 0.431 γ CCC($37)$ 74 A 168 186 168 0.454 1.440 186 167 0.400 1.285 γ CCC(41) 75 A A 130 116 0.543 2.998 128 118 0.596 2.901 γ CCC(41) 76 A<	64	А		441	449	443	5.371	0.187	447	441	2.706	0.215	γC-O(46)
66 A 407 391 52.349 2.237 402 390 6.308 1.576 γ C-0(42) 67 A 397 382 49.349 1.447 389 380 4.868 2.464 γ C-0(43) 68 A 374 390 373 4.639 3.066 362 369 3.958 2.327 γ CC(40) 69 A 317 330 315 0.732 2.212 329 316 86.986 1.660 γ OH(46) 70 A 294 308 297 2.872 0.595 306 294 2.949 0.606 γ OH(51) 71 A 271 292 273 0.842 1.726 271 2.71 2.289 1.841 γ C=0(41) 72 A 237 245 237 1.146 0.884 243 236 0.891 0.638 γ C=0(42) 73 A 179 199 18	65	А		408	419	407	5.983	0.241	416	406	7.843	0.298	γC-O(43)
67 A 397 382 49.349 1.447 389 380 4.868 2.464 γ C-Q(43) 68 A 374 390 373 4.639 3.066 362 369 3.958 2.327 γ CCC(40) 69 A 317 330 315 0.732 2.212 329 316 86.986 1.660 γ OH(46) 70 A 294 308 297 2.872 0.595 306 294 2.949 0.606 γ OH(45) 71 A 271 292 273 0.842 1.726 271 2.718 2.891 1.841 γ C-O(41) 72 A 237 245 237 1.146 0.884 243 236 0.891 0.638 γ C-O(4) 73 A 179 199 180 2.440 0.420 197 178 2.466 0.431 γ CCC(37) 74 A 168 186 168 0.454 1.440 186 167 0.400 1.285 γ CC(66	А			407	391	52.349	2.237	402	390	6.308	1.576	γC-O(42)
68 A 374 390 373 4.639 3.066 362 369 3.958 2.327 yCCC(40) 69 A 317 330 315 0.732 2.212 329 316 86.986 1.660 yOH(46) 70 A 294 308 297 2.872 0.595 306 294 2.949 0.606 yOH(45) 71 A 271 292 273 0.842 1.726 271 271 2.289 1.841 yC=0(41) 72 A 237 245 237 1.146 0.884 243 236 0.891 0.638 yC=0(42) 73 A 179 199 180 2.440 0.420 197 178 2.466 0.431 yCCC(37) 74 A 168 168 0.653 2.998 128 118 0.596 2.901 yCCC(41) 76 A 121 106 <	67	А			397	382	49.349	1.447	389	380	4.868	2.464	γC-O(43)
69A3173303150.7322.21232931686.9861.660yOH(46)70A2943082972.8720.5953062942.9490.606yOH(51)71A2712922730.8421.7262712712.2891.841yC=0(41)72A2372452371.1460.8842432360.8910.638yC=0(42)73A1791991802.4400.4201971782.4660.431yCC(37)74A1681861680.4541.4401861670.4001.285yCC(46)75A1211060.4722.1351181070.7692.212yCC(41)76A1211060.4722.1351181070.7692.212yCC(47)77A58550.9173.07959561.1113.251yCC(52)79A58550.9173.07959561.1113.251yCC(58)80A61631301.8200.59933321.8201.767yCC(46)81A6661666.559.23617160.4538.792yCC(43)	68	А		374	390	373	4.639	3.066	362	369	3.958	2.327	γCCC(40)
70A2943082972.8720.5953062942.9490.606 γ OH(51)71A2712922730.8421.7262712712.2891.841 γ C=0(41)72A2372452371.1460.8842432360.8910.638 γ C=0(42)73A1791991802.4400.4201971782.4660.431 γ CCC(37)74A1681861680.4541.4401861670.4001.285 γ CCC(46)75A1301160.5432.9981281180.5962.901 γ CCC(41)76A1211060.4722.1351181070.7692.212 γ CCC(47)77A58550.9173.07959561.1113.251 γ CCC(52)79A31301.8200.59933321.8201.767 γ CCC(46)81A16160.3539.23617160.4538.792 γ CCC(43)	69	А		317	330	315	0.732	2.212	329	316	86.986	1.660	γOH(46)
71A2712922730.8421.7262712712.2891.841 γ C=0(41)72A2372452371.1460.8842432360.8910.638 γ C=0(42)73A1791991802.4400.4201971782.4660.431 γ CCC(37)74A1681681680.4541.4401861670.4001.285 γ CCC(46)75A11100.5432.9981281180.5962.901 γ CCC(41)76A11211060.4722.1351181070.7692.212 γ CCC(47)77A78743.0810.62883782.7110.594 γ CCC(49)78A58550.9173.07959561.1113.251 γ CCC(52)79A31301.8200.59933321.8201.767 γ CCC(46)81A16160.3539.23617160.4538.792 γ CCC(43)	70	А		294	308	297	2.872	0.595	306	294	2.949	0.606	γOH(51)
72A2372452371.1460.8842432360.8910.638 γ C=0(42)73A1791991802.4400.4201971782.4660.431 γ CCC(37)74A1681681680.4541.4401861670.4001.285 γ CCC(46)75A11301160.5432.9981281180.5962.901 γ CCC(41)76A11211060.4722.1351181070.7692.212 γ CCC(47)77A78743.0810.62883782.7110.594 γ CCC(49)78A58550.9173.07959561.1113.251 γ CCC(52)79A31301.8200.59933321.8201.767 γ CCC(46)81A16160.3539.23617160.4538.792 γ CCC(43)	71	А		271	292	273	0.842	1.726	271	271	2.289	1.841	γC=O(41)
73 A 179 199 180 2.440 0.420 197 178 2.466 0.431 γCCC(37) 74 A 168 186 168 0.454 1.440 186 167 0.400 1.285 γCCC(46) 75 A 10 130 116 0.543 2.998 128 118 0.596 2.901 γCCC(41) 76 A 121 106 0.472 2.135 118 107 0.769 2.212 γCCC(47) 77 A 10 74 3.081 0.628 83 78 2.711 0.594 γCCC(49) 78 A 10 58 55 0.917 3.079 59 56 1.111 3.251 γCCC(52) 79 A 10 31 30 1.820 0.599 33 32 1.820 1.767 γCCC(46) 80 A 16 16 0.353 9.236	72	А		237	245	237	1.146	0.884	243	236	0.891	0.638	γC=O(42)
74A1681861680.4541.4401861670.4001.285γCC(46)75A1301160.5432.9981281180.5962.901γCC(41)76A1211060.4722.1351181070.7692.212γCC(47)77A78743.0810.62883782.7110.594γCC(49)78A58550.9173.07959561.1113.251γCC(52)79A34331.2232.84336340.8541.773γCC(58)80A61160.3539.23617160.4538.792γCC(43)	73	А		179	199	180	2.440	0.420	197	178	2.466	0.431	γCCC(37)
75A1301160.5432.9981281180.5962.901γCC(41)76A1211060.4722.1351181070.7692.212γCC(47)77A78743.0810.62883782.7110.594γCC(49)78A58550.9173.07959561.1113.251γCC(52)79A34331.2232.84336340.8541.773γCC(58)80A31301.8200.59933321.8201.767γCC(46)81A16160.3539.23617160.4538.792γCC(43)	74	А		168	186	168	0.454	1.440	186	167	0.400	1.285	γCCC(46)
76 A 121 106 0.472 2.135 118 107 0.769 2.212 γCCC(47) 77 A 78 74 3.081 0.628 83 78 2.711 0.594 γCCC(49) 78 A 58 55 0.917 3.079 59 56 1.111 3.251 γCCC(52) 79 A 34 33 1.223 2.843 36 34 0.854 1.773 γCCC(58) 80 A 31 30 1.820 0.599 33 32 1.820 1.767 γCCC(43) 81 A 16 16 0.353 9.236 17 16 0.453 8.792 γCCC(43)	75	А			130	116	0.543	2.998	128	118	0.596	2.901	γCCC(41)
77 A 78 74 3.081 0.628 83 78 2.711 0.594 γCCC(49) 78 A 58 55 0.917 3.079 59 56 1.111 3.251 γCCC(52) 79 A 34 33 1.223 2.843 36 34 0.854 1.773 γCCC(58) 80 A 31 30 1.820 0.599 33 32 1.820 1.767 γCCC(43) 81 A 16 16 0.353 9.236 17 16 0.453 8.792 γCCC(43)	76	А			121	106	0.472	2.135	118	107	0.769	2.212	γCCC(47)
78 A 58 55 0.917 3.079 59 56 1.111 3.251 γCCC(52) 79 A 34 33 1.223 2.843 36 34 0.854 1.773 γCCC(58) 80 A 31 30 1.820 0.599 33 32 1.820 1.767 γCCC(46) 81 A 16 16 0.353 9.236 17 16 0.453 8.792 γCCC(43)	77	А			78	74	3.081	0.628	83	78	2.711	0.594	γCCC(49)
79 A 34 33 1.223 2.843 36 34 0.854 1.773 γCCC(58) 80 A 31 30 1.820 0.599 33 32 1.820 1.767 γCCC(46) 81 A 16 16 0.353 9.236 17 16 0.453 8.792 γCCC(43)	78	А			58	55	0.917	3.079	59	56	1.111	3.251	$\gamma CCC(52)$
80 A 31 30 1.820 0.599 33 32 1.820 1.767 γCCC(46) 81 A 16 16 0.353 9.236 17 16 0.453 8.792 γCCC(43)	79	А			34	33	1.223	2.843	36	34	0.854	1.773	γCCC(58)
81 A 16 16 0.353 9.236 17 16 0.453 8.792 γCCC(43)	80	А			31	30	1.820	0.599	33	32	1.820	1.767	γCCC(46)
	81	А			16	16	0.353	9.236	17	16	0.453	8.792	γCCC(43)

ass-asym. stretching, ss-sym.stretching, ipb-in-plane-bending, opb-out-of-plane bending, sb-sym. bending, ipr-in-plane rocking, opr-out-of-plane rocking, sciss-scissoring, rock-rocking, wagg-wagging, twist-twisting. Assignments: v-stretching, β -in-plane bending, γ -out-of-plane bending.

C-H vibration

Aromatic structure shows the presence of the C-H stretching vibration in the range3100-3000 cm-1, due to aromatic C-H stretching vibrations. The observed wave numbers of C-H stretching vibration are also good agreement with the measured values and literature data [15-17]. The C-H in-plane and out-of-plane bending vibration generally in the region 1300-1000 cm-1 and 1000-700 cm-1 [[18], respectively. The FT-IR bands at 3466, 2933, 2866 cm-1 and FT-Raman bands at 3071 cm-1 are assigned to C-H vibration. As showed by the PED, these three modes involve approximately 100% contribution sagged that they are pure C-H stretching modes. The C-H In plane bending vibration computed at 1244, 1199, 1166, 1333, 1099, 1063, 1022 cm-1 by B3LYP/6-31+G (d) and B3LYP/6-311++G (d, p) FT-IR The corresponding theoretically computed values are presented in Table 2.

C=O vibration

The Carbonyl group vibration in ketenes are best characteristics band in vibrational spectra, and for this reason, such bands have been subject of extensive studies. The stretching vibration in the band region at 1700-1800 cm⁻¹. Also the koczon'et al. [19], the C=O in-plane and out-of-plane bending vibration is found at 952 cm⁻¹ and 263 cm⁻¹. The FT-IR and FT-Raman vibrational bond at 1744, 1678 cm⁻¹ and 1672 cm⁻¹. The C=O stretching vibration in OSPA has a main contribution in the modes, with B3LYP/6-31+G (d) and 6-311++G (d, p) methods show good aggrement with literature value [20].

C-O vibration

The carbonyl groups generally absorb in the spectral region 1300-1000 cm⁻¹ [21]. C-O stretching vibration is assigned at In the region below 1500 cm⁻¹ is called fingerprint region. The characteristics band of C-O stretching vibration appears in the region is mixed with C-C stretching mode C-C ring torsion and C-C-H bending mode. We can find that the C-O vibration has been calculated by neighboring molecular interaction. The C-O in-plane and out-of-plane bending vibration is 842-798 cm⁻¹ and 404-399 cm⁻¹. The FT-IR and FT-Raman bands at 1300, 1277 cm⁻¹ and 1302, 1255 cm⁻¹ respectively.

C-C vibration

The aromatic carbon-carbon (C-C) stretching vibration occurs in the region1625-1430 cm⁻¹ [22]. In general, the bands are variable intensity and are observed at 1625-1590, 1590-1575, 1540-1470, 1465-1430, and 1380-1280 cm⁻¹ from the frequency ranges given by Varsanyi [23] Therefore, the C-C stretching vibrations found at 1611, 1577, 1466, 1411, 1376, 1333 cm⁻¹ in FT-IR and 1627, 1593, 1453, 1377 cm⁻¹ in the FT-Raman spectrum the PED values. These C-C ring inplane bending vibration is occurs in the region 840 and 270 cm⁻¹, the ring out of-plane bending vibration banding modes of OSBA are also listed in Table 2. The theoretically computed values for C-C vibrational modes by B3LYP/6-31+G (d) and 6-311++G (d, p) method give excellent agreement with experimental data. The remaining vibration like CCC in-plane and out-of-plane bending vibrations are assigned with reference to the literature data are presented in Table 2.

O-H vibration

The O-H group gives rise to three vibration (stretching, in-plane and out-plane bending vibrations). The unbounded or free hydroxyl group of alcohol and phenols absorb strongly in the region $3550-3200 \text{ cm}^{-1}$ [24]. The O-H in-plane bending

vibrationis 1150-1250 cm⁻¹ and out-plane bending vibration is 320-290 cm⁻¹. of alcohol and phenols absorb strongly in the region 3650-3584 cm⁻¹ sharp free hydroxyl bands are observed only in the vapor phase or in very dilute solution in non-polar solvents. The O-H group vibration are likely to be the most sensitive's to the environment, so they show pronounced shift in the spectra of hydrogen–bonded species. In your study FT-IR band at 3466 cm⁻¹ have been assigned to O-H stretching vibration with maximum PED contributing 100%. A comparison of these bands with that of the computed values by B3LYP/6-31+G (d) and B3LYP/6-311++G (d, p) methods.

4.3 MULLIKEN'S ATOMIC CHARGE

In Mulliken's analysis, half the overlap population is assigned to each contributing orbital, giving the total population of each atomic orbital. Summing overall the atomic orbital on a specific atom gives as the gross atomic population. The sum of all net and overlap population equals the total numbers of electron in the molecule. The charge distribution calculated by the Mulliken [25]. The charge distribution on the molecule has an important inference on the vibrational spectra [26]. The values of the Mulliken's atomic charges of an each atoms for the title compound wave also obtained with the help of B3LYP levels of theory incorporating 6-31+G (d) and 6-311++G (d, p)basis set. The Mulliken's atomic charges on each atom of the title compound are presented in *Table 3*. And the graphical representation is shown in Fig. 4.

Table 3. Mullikan's population analysis of O-(Salicyloyloxy) benzoic acid at B3LYP/6-31+G (d) and P3LVP/6 311 + C (d, p) methods

	Mullikan'	s atomic charge
Atom	F	B3LYP
INO.	6-31+G	6-311++G (d,
	(d)	p)
C_1	-0.732	-0.891
C_2	0.471	1.129
C ₃	-0.218	0.013
C_4	0.001	-0.171
C ₅	-0.204	-0.383
C ₆	0.225	0.201
C ₇	0.786	-0.011
O_8	-0.474	-0.279
O_9	-0.657	-0.232
H_{10}	0.543	0.305
H_{11}	0.227	0.216
H ₁₂	0.189	0.173
H ₁₃	0.190	0.174
H_{14}	0.197	0.172
O ₁₅	-0.142	0.269
C ₁₆	-0.208	-0.880
O ₁₇	-0.290	-0.068
C ₁₈	0.693	0.886
C ₁₉	-0.233	-0.208
C ₂₀	0.025	-0.194
C ₂₁	-0.426	-0.241
C ₂₂	-0.304	-0.431
C ₂₃	-0.275	-0.280
O ₂₄	-0.645	-0.186
H ₂₅	0.504	0.269
H ₂₆	0.169	0.129
H ₂₇	0.187	0.166
H ₂₈	0.185	0.179
H ₂₉	0.218	0.175

50299

Table 4 .The electric dipole moment (μ) (debye), the mean polarizability (α) (e.s.u.), anistropic polarizability ($\Delta \alpha$) (e.s.u.) and first hyper polarizability (β_{tot}) (e.s.u) for O-(Salicyloyloxy) benzoic acid at B3LYP/6-31+G (d) and

BSLYP/0	5-311++ G (a,	, p) methods.
Paramet	B3LYP/63	B3LYP/6311
ers	1+G (d)	++G (d , p)
μ_x	-2.174	-2.172
μ_{v}	-1.051	-1.050
μ_z	0.004	-0.004
μ	2.4529	2.6127
α_{xx}	243.740	245.270
α_{xy}	30.671	31.147
α_{vv}	234.209	235.775
α_{xz}	0.032	0.031
α_{vz}	0.181	0.182
α_{zz}	91.668	92.447
α	189.8723	197.1637
Δα	-894.311	-882.4697
β_{xxx}	-484.463	-509.557
β_{xxy}	-265.380	-284.496
β_{xyy}	168.573	156.306
β_{yyy}	-246.188	-248.997
β_{xxz}	0.591	0.721
β_{xyz}	0.914	0.883
β_{yyz}	0.599	0.692
β_{xzz}	-12.733	-12.656
β_{yzz}	9.134	10.819
β_{zzz}	-0.823	-0.787
β_{tot}	4.54 x10 ⁻	5.33x10 ⁻
	³⁰ e.s.u	³⁰ e.s.u





The polarizability (α), hyperpolarizability (β) and electric dipole moment (μ) the OSBA are calculated by finite method using B3LYP method with 6-31+G (d) and 6-311++G (d, p) basis set and are presented in the Table 4. To calculate the electric dipole moment and the first hyperpolarizability tensor components for a given system will depend on the choice of the Cartesian co-ordinate system. (x, y, z) = (0, 0, 0) was chosen a own of mass of molecule. The polarizability of this novel molecule system for which $\alpha_{xxx} = \alpha_{yyy} = \alpha_{zzz}$ is said to be isotropic. The polarizability is isotropic is the same in all direction for a molecular system whose electron density is spherically symmetrical. If the molecule is perfectly isotropic (P) and (E) will have the same direction and is then simple scaler quantity. The polarizability of this novel molecular system for which $\alpha_{xxx} \neq \alpha_{yyy} \neq \alpha_{zzz}$ will no longer have the same direction (E). The first hyperpolarizability (β_{total}) and related properties (α , β and $\Delta \alpha$) are calculated and it's based on the finet field approach. In the presence of an external electric field. First huperpolarizability is third rank tensor that can be described by a 3*3*3 matrix. The 29 components of the 3D matrix can be reduced of the kleinman symmetry [27]. It can be given in the lower tetrahedral format. It is obvious that the lower port of the 3*3*3 matrixes is a tetrahedral. The components of the β are defined as the coefficient in the taylor series expansion of energy in an external electric field. The external electric field is weak and homogeneous this expansion becomes as follows.

$$E = E^{0} - \frac{\mu_{i}F_{i}}{1!} - \frac{\alpha_{ij}F_{i}F_{j}}{2!} - \frac{\beta_{ijk}F_{i}F_{j}F_{k}}{3!} - \frac{\gamma_{ijkl}F_{i}F_{j}F_{k}F_{l}}{4!} + \cdots$$

Where E° is the energy of the unperturbed molecules. F_{α} is the field at the orgin, and μ_{i} , α_{ij} , β_{ijk} are the component of dipole moment, polarizability and the first hyper polrizability respectively.

The total static dipole moment is

$$\mu = (\mu_x^2 + \mu_y^2 + \mu_z^2)^2$$

The polarizability anisotropy invariant is
$$\Delta \alpha = 2^{-\frac{1}{2}} [(\alpha_z - \alpha_z)^2 + (\alpha_z - \alpha_z)^2 + (\alpha_z - \alpha_z)^2 + 6\alpha_z^2]^{\frac{1}{2}}$$

The average hyperpolarizability

$$\beta_{tot} = (\beta_x^2 + \beta_y^2 + \beta_z^2)^{\frac{1}{2}}$$

Where
$$\beta_x = (\beta_{xxx} + \beta_{xyy} + \beta_{xzz})$$

$$\beta_{y} = (\beta_{yyy} + \beta_{xxy} + \beta_{yzz})$$

 $\beta_z = (\beta_{zzz} + \beta_{xxz} + \beta_{yyz})$

Where α_{xx} , α_{yy} , and α_{zz} are tensor components of polarizability. β_x , β_y and β_z are tensor components of hyperpolarizability. Since the value of polarizability and hyper polarizability of the GAUSSIAN 09 output are reported in atomic units (a.u.), the calculated values have been converted in to electrostatic units (*e.s.u.*) (1 a.u. =8.639x10⁻³³ e.s.u.). The total molecular dipole moment, polarizability and first hyper polarizability are 2.4529 Debye, -894.311 x 10⁻³³ e.s.u. and 4.54 x10⁻³⁰ e.s.u. in B3LYP/6-31+G (d) and 2.6127 debye, -882.4697 x 10⁻³³ e.s.u. and 5.33 x10⁻³⁰ e.s.u. in B3LYP/6-311++G (d, p) methods, respectively

4.5 HOMO-LUMO

The HOMO-LUMO analysis for OSPA was conducted by B3LYP/6-31+G (d) and B3LYP/6-311++G (d, p) level of theory. Using HOMO and LUMO energies and quantum chemical parameters [29]. Many organic molecules that containing conjugated π electrons are characterized and analyzed by means of vibrational spectroscopy [29]. HOMO is a Highest occupy molecular orbital's and LUMO is a lowest unoccupied molecular orbital's. HOMO which can be through the outer most orbital containing the donor electron. On the other hand LUMO can be through the inner most orbital containing free place to accept electrons. Therefore, while the energy of the HOMO is directly related to the ionization potential, LUMO energy is directly related to the electron affinity. The atomic orbital compositions of the frontier molecular orbital are shown in Fig. 5. Energy difference between HOMO and LUMO orbital is called as energy gap that is an important stability for structures. HOMO and LUMO values are calculated by B3LYP/6-31+G (d) and B3LYP/6-311++G (d, p) methods are given in Table 5.

Tabl	e 5.Compar	ison of H	OMO, LU B3I	MO energy LYP/6-31+0	gaps and b G (d) and B	related mol 3LYP/6-31	lecular prop 1++G (d, p)	oerties of (methods)	O-(Salicyloy	vloxy) benzoic ac	id at
	Mologular	Enorm	Energy	Ionisation	Electron	Global	Electro	Global	Chemical	Global	

Molecular properties	Energy (eV)	Energy gap (eV)	Ionisation potential (I)	Electron affinity (A)	Global Hardnes s (η)	Electro negativity (χ)	Global softnes s (v)	Chemical potential (µ)	Global Electrophilicit y (ω)			
				B3LY	P/6-31+G (d	l)						
HOMO	-6.7080	4 0226	6 7080	1 7954	2 4612	4 2467	0 4062	1 2467	2 6626			
LUMO	-1.7854	4.9220	4.9220	4.9220	0.7080	1.7654	2.4015	4.2407	0.4005	-4.2407	3.0030	
				B3LYP/	6-311++G (d	l, p)						
HOMO	-6.7630	4 0297	6 7620	1 9242	2 4644	4 2087	0 4059	4 2087	2 7401			
LUMO	-1.8343	4.9207	0.7050	1.6343	2.4044	4.2907	0.4038	-4.2967	5.7491			

The TDOS, PDOS and overlap population density of states, in terms of Mulliken population analysis were calculated and created by convoluting the molecular orbital information with Gaussian curves of unit height and a full width t half maximum of 0.3 eV using Gaussum 2.2. The main used of the DOS plots is to provide pictorial representation molecular orbital compositions and their contributions to chemical bonding through the PDOS plots which are also referred in the literature as crystal orbital overlab population diagram. The density of electronic states has been calculated and they are displayed for the Figs. 6 and 7.



Fig 5. The molecular orbitals and energies for the HOMO and LUMO of O-(Salicyloyloxy) benzoicacid.



(Salicyloyloxy) benzoicacid.



Fig 7. The calculate TDOS diagram of O-(Salicyloyloxy) benzoicacid.

4.6. MOLECULAR ELECTROSTATIC POTENTIAL (MEP)

Electrostatic potential maps, also known as electrostatic potential energy maps, or molecular electrical potential surfaces, illustrative the charge distributions of molecules three dimensionally. The purpose of finding the electrostatic potential is to find the reactive site of a molecule. Knowledge of the charge distribution can be used to determine how molecules interact with one another. The molecular electrostatic potential surfaces (MEPs) for OSBA are shown in Fig. 8. The molecular electrostatic potential surface MEP which is a 3D plot of electrostatic potential mapped on to the iso-electron density surface simultaneously display molecular shape, size and electrostatic potential values. The color scheme for the MEPs surface is red electron (O_8) rich or partially negative charge; blue -electron (H₁₀, H₂₅) deficient or partially positive charge; light blue-slightly electron deficient region; yellow slightly electron rich region, respectively.



Fig 8. The total electron density surface mapped with of O-(Salicyloyloxy) benzoicacid.

CONCLUSION

The FT-IR and FT-Raman spectra of OSBA were carried out for the first time. A complete vibrational and molecular structural analysis has been performed based on the quantum mechanical approach by DFT calculation. The equilibrium geometrical and harmonic frequencies were determined and analyzed for the most stable structure using B3LYP levels with 6-31+G (d) and 6-311++G (d, p) basis sets, and these results compared with X-ray crystal data, and experimental spectra of the molecule. Therefore the assignments with reasonable deviation from the experimental value seem to be correct. The study demonstrates the scaled calculations are powerful approach for understanding the vibrational spectra of the title molecule. The calculated HOMO and LUMO energy gap are confirm the presence of charge transfer within the molecule. The HOMO and LUMO energies can be used to estimate the ionization potential, electron affinity, electro negativity, electrophilicity index, global hardness, softness and chemical potential of the molecule. The predicted molecular electrostatic potential shows that this molecule has several possible sites for electrophilic attack in which V(r)calculations provide insights into the order of presence. REFERENCES

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50301