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Molecular Structure, Vibrational Spectral Studies and NLO Properties of 4-Benzyloxy-3-Methoxy-Benzaldehyde by DFT

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Abstract: Benzaldehydes and its derivatives are the simplest in aromatic aldehydes and have wide range of use in different industries, they also exhibits different biological activities. Due to this reason there exist a vast field of study of substituted benzaldehydes. In the present study 4-benzyloxy3-methoxy-benzaldehyde is taken for study. The spectral studies were performed for FTIR, IR (KBr and Nuzol) and Raman. Quantum mechanical calculations of geometries, energies, vibrational wave numbers and thermodynamic constants have been performed with Gaussian 09W program package using the Becke-3Lee-Yang-Parr (B3LYP) functional supplemented with the standard 6-31G (DP). The optimised geometrical parameters obtained by computational method used shows good agreement with the experimental data. The thermodynamic properties as heat capacity, entropy, enthalpy and Gibb's free energy of the titled compounds at different temperatures were also calculated along with dipole moment, polarisability and hyperpolarisability.

Keywords: 4-benzyloxy3-methoxy-benzaldehyde, vibrational, NLO, Gaussian 09W, DFT/ B3LYP ,thermodynamic parameters, FTIR, dipole moment, polarisability, hyperpolarisability.

I. INTRODUCTION

Spectroscopic studies of the benzaldehyde and their derivatives have been carried out as the vibrational spectra are very useful for understanding of specific biological activities and for the analysis of relatively complex system. Benzaldehydes have a large usage in different industries as perfumes, flavouring compounds , soaps , foods, preparations of some aniline dyes , solvent for oils etc.[1]. They have also shown anti tumour activity in mice [1,2]. In this light lots of aspects of substituted benzaldehydes and its derivatives are unexplored in spite of the fact that much work has been done on these compounds.[3-6].

II. EXPERIMENTAL

Spec-pure grade sample of 4-benzyloxy-3-methoxy- benzaldehyde (abbreviated and further mentioned as BMB) was obtained from M/S Aldrich Chemie, West Germany. The Purity of sample was confirmed by elemental analysis and melting point determination. The laser Raman spectra of both the molecules were recorded on Spex Rama Lab spectrophotometer using 52 MW Argon-Krypton laser beam of wavelength 488 nm. The infrared spectra of these two compounds were recorded on Perkin Elmer spectrophotometer model -52 in the region 400-4000 cm^{-1} using KBr and nuzol technique.

III. COMPUTATIONAL

All the calculations were carried out for BMB with Gaussian 03W program package [7]using the Becke-3Lee-Yang-Parr (B3LYP) functional supplemented with the standard 6-31G(DP) basis set further referred as DFT calculations. All the parameters were allowed to relax and all the calculations converged to an optimized geometry which corresponds to a true energy minimum, as revealed by the absence of imaginary values in the wave number calculations.

IV. RESULTS AND DISCUSSION

A. *Molecular Structure*

The molecular structure of the mentioned compound BMB is shown in Figure 1. The optimized bond lengths, bond angles and dihedral angles of the compound is calculated by B3LYP method using B3LYP 6-311++G (d) and 6-311++G (D,P) basis sets are listed in Table 1 is in accordance with atom numbering scheme as shown in Fig. 1. Since the exact crystal structure of the compound BMB is not available till now, the optimized structure can only be compared with other similar system for which the crystal structures have been solved. [8]

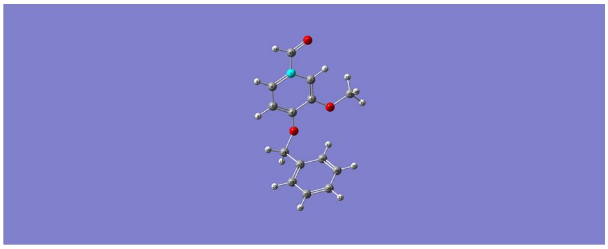


Figure 1

Calculated Optimized Geometrical Parameters of BMB, at B3LYP/6-31G(d,p): bond length (Å), bond angle(^{o}), dihedral angles(^{o})

S. No	Atoms of molecule	Bond length (Å)	Angle between atoms (^{o})	Bond angle (^{o})	Dihedral angle between atoms (^{o})	Dihedral angle (^{o})
1.	R(1,2)	1.3952	A(2,1,6)	119.9985	D(6,1,2,3)	0.0323
2.	R(1,6)	1.3948	A(2,1,10)	119.9972	D(6,1,2,7)	179.9532
3.	R(1,10)	1.54	A(6,1,10)	120.0043	D(10,1,2,3)	-179.9729
4.	R(2,3)	1.3947	A(1,2,3)	120.0086	D(10,1,2,7)	-0.052
5.	R(2,7)	1.0997	A(1,2,7)	119.9808	D(2,1,6,5)	0.0149
6.	R(3,4)	1.3954	A(3,2,7)	120.0106	D(2,1,6,9)	179.9892
7.	R(3,28)	1.43	A(2,3,4)	119.9942	D(10,1,6,5)	-179.9798
8.	R(4,5)	1.3948	A(2,3,28)	120.0128	D(10,1,6,9)	-0.0056
9.	R(4,13)	1.43	A(4,3,28)	119.993	D(2,1,10,11)	-89.9606
10.	R(5,6)	1.3951	A(3,4,5)	119.994	D(2,1,10,12)	90.0394
11.	R(5,8)	1.0998	A(3,4,13)	119.9811	D(6,1,10,11)	90.0341
12.	R(6,9)	1.0996	A(5,4,13)	120.0249	D(6,1,10,12)	-89.9659
13.	R(10,11)	1.07	A(4,5,6)	120.0047	D(1,2,3,4)	-0.0568
14.	R(10,12)	1.2584	A(4,5,8)	120.0113	D(1,2,3,28)	179.9619
15.	R(13,14)	1.43	A(6,5,8)	119.984	D(7,2,3,4)	-179.9777
16.	R(14,15)	1.07	A(1,6,5)	120.0	D(7,2,3,28)	0.041
17.	R(14,16)	1.07	A(1,6,9)	120.008	D(2,3,4,5)	0.0341
18.	R(14,17)	1.54	A(5,6,9)	119.992	D(2,3,4,13)	-179.9964
19.	R(17,18)	1.3952	A(1,10,11)	119.8865	D(28,3,4,5)	-179.9846
20.	R(17,19)	1.3948	A(1,10,12)	120.2269	D(28,3,4,13)	-0.0151
21.	R(18,20)	1.3947	A(11,10,12)	119.8865	D(2,3,28,29)	-61.5726
22.	R(18,21)	1.0997	A(4,13,14)	109.5	D(4,3,28,29)	118.4461
23.	R(19,22)	1.3951	A(13,14,15)	109.4712	D(3,4,5,6)	0.0131
24.	R(19,23)	1.0996	A(13,14,16)	109.4712	D(3,4,5,8)	-179.9995
25.	R(20,24)	1.3954	A(13,14,17)	109.4712	D(13,4,5,6)	-179.9563
26.	R(20,25)	1.0997	A(15,14,16)	109.4712	D(13,4,5,8)	0.0311
27.	R(22,24)	1.3948	A(15,14,17)	109.4713	D(3,4,13,14)	90.1178
28.	R(22,26)	1.0998	A(16,14,17)	109.4712	D(5,4,13,14)	-89.9127
29.	R(24,27)	1.0997	A(14,17,18)	119.9972	D(4,5,6,1)	-0.0376
30.	R(28,29)	1.43	A(14,17,19)	120.0043	D(4,5,6,9)	179.9881
31.	R(29,30)	1.07	A(18,17,19)	119.9985	D(8,5,6,1)	179.975

32.	R(29,31)	1.07	A(17,18,20)	120.0086	D(8,5,6,9)	0.0007
33.	R(29,32)	1.07	A(17,18,21)	119.9808	D(4,13,14,15)	-179.9071
34.			A(20,18,21)	120.0106	D(4,13,14,16)	60.0929
35.			A(17,19,22)	120.0	D(4,13,14,17)	-59.9071
36.			A(17,19,23)	120.008	D(13,14,17,18)	-57.8579
37.			A(22,19,23)	119.992	D(13,14,17,19)	122.1368
38.			A(18,20,24)	119.9942	D(15,14,17,18)	62.142
39.			A(18,20,25)	120.0128	D(15,14,17,19)	-117.8632
40.			A(24,20,25)	119.993	D(16,14,17,18)	-177.8579
41.			A(19,22,24)	120.0047	D(16,14,17,19)	2.1368
42.			A(19,22,26)	119.984	D(14,17,18,20)	-179.9729
43.			A(24,22,26)	120.0113	D(14,17,18,21)	-0.052
44.			A(20,24,22)	119.994	D(19,17,18,20)	0.0323
45.			A(20,24,27)	119.9811	D(19,17,18,21)	179.9532
46.			A(22,24,27)	120.0249	D(14,17,19,22)	-179.9798
47.			A(3,28,29)	109.5	D(14,17,19,23)	-0.0056
48.			A(28,29,30)	109.4712	D(18,17,19,22)	0.0149
49.			A(28,29,31)	109.4712	D(18,17,19,23)	179.9892
50.			A(28,29,32)	109.4712	D(17,18,20,24)	-0.0568
51.			A(30,29,31)	109.4713	D(17,18,20,25)	179.9619
52.			A(30,29,32)	109.4712	D(21,18,20,24)	-179.9777
53.			A(31,29,32)	109.4712	D(21,18,20,25)	0.041
54.					D(17,19,22,24)	-0.0376
55.					D(17,19,22,26)	179.975
56.					D(23,19,22,24)	179.9881
57.					D(23,19,22,26)	0.0007
58.					D(18,20,24,22)	0.0341
59.					D(18,20,24,27)	-179.9964
60.					D(25,20,24,22)	-179.9846
61.					D(25,20,24,27)	-0.0151
62.					D(19,22,24,20)	0.0131
63.					D(19,22,24,27)	-179.9563
64.					D(26,22,24,20)	-179.9995
65.					D(26,22,24,27)	0.031
66.					D(3,28,29,30)	82.8463
67.					D(3,28,29,31)	-157.1537
68.					D(3,28,29,32)	-37.1537

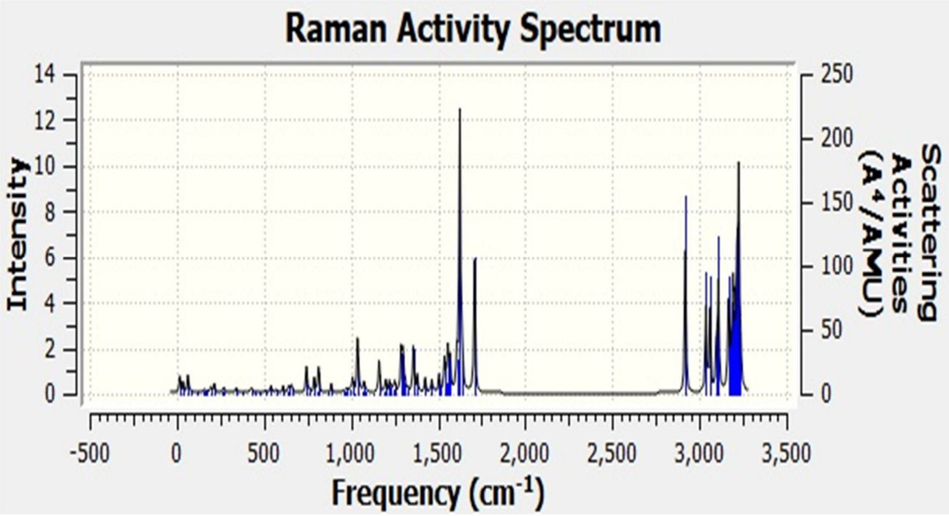
B. Vibrational Spectra

A detailed study of vibrational spectra has been carried out of the reported compound BMB and its vibrational frequencies have been calculated using DFT-B3LYP level with 6-31++G(d,p), there is a good agreement between the observed frequencies and those calculated by the DFT comparative chart is shown in Table 2 in which experimental values of IR (KBr and nuzol), FTIR and laser Raman are displayed and simultaneously compared with the calculated values , respective assignments are shown corresponding to the results.

S.No	Calculated Frequencies			Experimental Frequencies				Assignments
	Frequency	I R	Raman Activity	Raman	IR(KBr)	IR(Nuzol)	FTIR	
1	17.09	0.0838	9.5624					
2	37.56	0.6967	5.6534	40				
3	64.03	1.1422	9.5906		56.25			
4	77.57	5.2046	1.4154	75				
5	114.22	6.2968	1.0163	114				
6	152.91	6.6623	1.4414	154				
7	165.13	2.3527	1.1883	169				
8	171.78	1.1662	1.5369					
9	195.96	2.5564	3.8082					
10	215.01	3.5219	5.8225					
11	258.98	1.3437	0.85	238				
12	269.56	2.9908	1.8916					
13	272.8	5.1187	2.4645	306				
14	340.12	3.4819	3.3594					
15	373.86	6.8729	1.1237					
16	426.69	1.9839	2.9115		424	417		
17	432.62	0.5018	1.5374	445				
18	452.6	6.6319	1.4434			443		
19	477.72	7.434	0.9989		487			
20	514.01	6.5073	1.8561					
21	540.9	2.9829	5.163		533			
22	569.67	10.487	2.6541	571	562		562.9	
23	609.4	15.4741	3.8565	608	590			
24	634.98	6.6307	1.6844					
25	644.46	25.4521	4.8084					
26	659.33	0.546	5.3805	668	658	657	664.8	Benzyloxy group vib.
27	743.04	57.7397	7.5906		699	699	705.5	
28	745.55	2.9784	11.2749		729	729		
29	761.22	70.7589	2.0952	745	749	748		Benzyloxy group vib.
30	789.44	2.5475	9.8687					
31	804.77	5.1078	1.2201					

32	813.47	3.2565	17.0797	815	814	813	817.5	
33	865.34	39.3129	1.3033	864	857	856		
34	887.54	0.4559	5.7387		867	867		
35	955.7	3.8063	2.1931		920	919		
36	965.03	12.4567	1.292					
37	975.84	25.4283	3.3398	980				
38	997.25	20.7786	3.2851		995	990	990.7	
39	1008.69	57.4489	10.4585	1005				
40	1023.98	4.3347	0.1458	1014				
41	1036.71	7.1085	28.4108		1032	1032		
42	1039.62	45.9348	11.3857					
43	1042.32	36.0296	6.5537	1045				C-H deformaton
44	1064.74	5.0209	1.3458					
45	1073.87	2.1404	7.8017					
46	1087.3	2.6381	2.4975					
47	1126.33	6.8258	0.7527				1138.3	
48	1160.63	223.9749	15.3457	1045	1160	1159		
49	1162.31	12.583	9.1586					
50	1187.86	11.2875	1.5374					
51	1200.46	18.0193	8.3746	1207				
52	1220.74	2.9392	8.4896		1237	1237		
53	1231.31	0.1759	4.717					
54	1242.59	52.266	3.0441					
55	1251.33	15.8146	8.2501	1252	1262	1261	1265.6	
56	1287.27	205.8154	31.6724	1272	1276	1276		
57	1297.76	166.3352	29.8757					
58	1311.22	21.0317	9.0126					
59	1328.37	10.7704	3.433					
60	1357.5	18.7576	34.5632	1360	1348	1348		C-C stretching
61	1380.65	4.8473	13.8039	1396	1385	1380		C-C stretching
62	1420.17	2.9607	3.3444		1401	1400		C-C stretching
63	1426.19	50.7143	10.7557	1438	1426	1425		C-C stretching
64	1463.89	57.6602	10.5604	1463	1466	1464		C-C stretching

65	1505.68	0.0824	11.7542		1506	1505		C-C stretching
66	1509.28	18.7986	4.3621				1510	C-C stretching
67	1536.13	41.4531	25.8317	1521				C-C stretching
68	1548.45	110.4146	7.8764					
69	1553.55	25.7719	3.0702					
70	1555.79	11.4604	30.9381					
71	1569.12	22.1381	26.8488					
72	1607.8	55.618	27.1678	1596	1598	1597		C-C stretching
73	1618.84	13.6277	23.7543					
74	1624.98	100.5387	213.6456					
75	1638.63	3.3304	26.548	1678	1667	1673	1678.1	
76	1709.16	129.7607	106.4191	1709				
77	2919.55	156.1254	154.4829	2853	2840	2854	2849.2	C-H stretching
78	3037.79	31.6419	94.3443	2964	2950	2926		
79	3060.49	25.7204	91.2246	3025	3013			C-H stretching
80	3096.26	30.7167	49.2209	3076	3061			
81	3109.18	15.9513	123.3103					
82	3166.09	13.2202	91.7108					
83	3174.09	7.7454	47.9705					
84	3190.19	1.633	71.8359					
85	3193.4	5.9949	64.6025					
86	3200.91	23.6376	82.2171		3408	3450		
87	3215.59	8.6848	129.8019	4100	3651			
88	3225.19	25.563	134.344					
89	3225.96	11.3977	109.43					
90	3235.81	4.9312	49.0456					



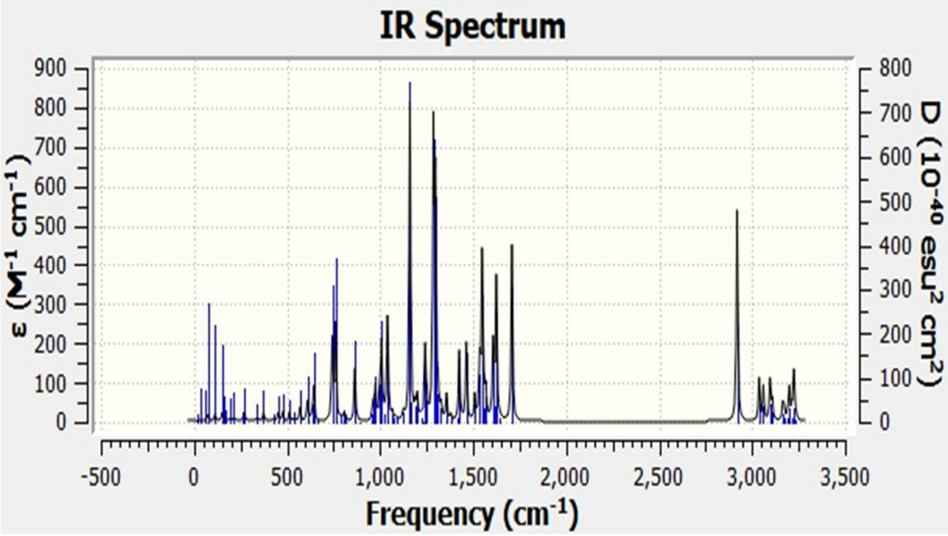


FIGURE 2

1) *C – H Vibrations:* In substituted benzene rings, the C-H stretching vibrations give rise to bands at 3120- 3000 cm-1[9]. In the present compound BMB these values are observed at 3025cm^{-1} and 3076 cm^{-1} for Raman and 3013cm^{-1} and 3061 cm^{-1} for IR(KBr). These values are in agreement with those obtained by DFT-B3LYP level with 6-31++G(d,p) which are 3060cm^{-1} and 3096 cm^{-1}. The in- plane aromatic C-H deformation vibrations occur in the region 1300-1000cm-1.[10] The vibrations at 1045cm^{-1} for Raman 1160 cm^{-1}and 1159 cm^{-1} for IR (KBr and nuzol respectively) and 1138.3 cm^{-1} for FTIR are in fair agreement with the calculated values i.e 1126,1160 and 1162 cm^{-1}.
2) *C – C vibrations:* The bands in the range 1400-1650 cm-1 are generally assigned to C-C stretching mode .[11] The bands of variable intensity are generally observed at 1625-1590 cm-1, 1590- 1575cm-1, 1540-1470cm-1, 1465- 1430cm-1 and 1380-1280cm-1 from the frequency ranges given by Varsanyi.[12] In the present study the bands observed at 1360, 1396, 1438, 1465, 1521, 1596 cm-1 at Raman, 1348, 1385, 1401, 1426, 1466, 1506, 1598 cm-1 at IR(KBr), 1348, 1380, 1400, 1425, 1464, 1505, 1597 cm-1 at IR (nuzol), and 1510 cm-1 in FTIR are assigned to C-C stretching mode. These values are in in good agreement with the calculated values of the compound which comes out to be at 1420.17, 1426.19, 1463.89, 1505.68, 1536.13, 1548.45, 1553.55, 1555.79, 1569.12, 1607.8, 1618.84, 1624.98 cm-1.
3) *Aldehyde group vibrations:* The C-H stretching vibrations of the aldehyde group usually appear in the region 2871–2806 cm-1 [13]. These are observed 2853cm-1 in Raman and 2840 cm-1 in IR (KBr) 2854 cm-1 in IR (nuzol) is in agreement with the calculated value which is 2919.55 and the literature values. The carbonyl C=O stretching vibrations in the substituted benzaldehydes are reported near 1700 cm_1 [13]. The bands cantered 1678.1 cm-1 in FTIR, 1667 cm-1 in IR (KBr) and 1673 (nuzol) and 1678 and 1709 cm-1 in Raman for BMB is attributed to C=O stretching vibration of the aldehyde group which shows fair agreement with the calculated value 1709.16. A weak-to-medium intensity band due to the aldehyde group CHO deformation vibration is found in the region 975–780 cm-1 [13] . In agreement with this, the bands at 815, 864, 980 cm-1 in Raman, 814, 857, 867, 920 cm-1 at IR(KBr), 813, 856, 867, 919 cm-1 at IR(nuzol) could be assigned to CHO out of plane deformation for BMB. These values shows support to the calculated values which is in the same given range and for the compound BMB are 789.44, 804.77, 813.47, 865.34, 887.54, 955.7, 965.03, 975.84 cm-1.
4) *Benzyloxy Group Vibrations:* The vibrations in the range 745-730 cm-1 and 700-695 cm-1 attributes to benzyloxy group.[14] The vibrations at 745 and 668 cm-1 at Raman, 749,729, 699, 658 cm-1 for IR(KBr), 657, 699, 729 and 748 cm-1 for IR(nuzol) and 664.8 and 705.5cm-1 for FTIR can be assigned to benzyloxy group. The calculated values for the same comes out to be 634.88, 644.46, 659.33, 743.04, 745.55 cm-1 . The experimental and the calculated values of frequency shows good agreement.

C. Thermodynamic Properties

Theoretical geometrical parameters represent a good approximation and they are the basis for calculating vibrational frequencies and thermodynamic parameters. The frequency calculations compute the zero point energies, thermal correction to internal energy and entropy as well as the heat capacity for a molecular system. These functions describe the thermodynamic stability of the system at the given conditions of pressure and temperature.

Zero-point correction = 0.258469 (Hartree/Particle)
Thermal correction to Energy = 0.273962
Thermal correction to Enthalpy = 0.274906
Thermal correction to Gibbs Free Energy = 0.213929
Sum of electronic and zero-point Energies = -800.984731
Sum of electronic and thermal Energies = -800.969239
Sum of electronic and thermal Enthalpies = -800.968295
Sum of electronic and thermal Free Energies = -801.029272

Table from calculation

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	171.914	59.343	128.338
Electronic	0	0	0
Translational	0.889	2.981	42.354
Rotational	0.889	2.981	33.467
Vibrational	170.136	53.381	52.517
Vibration 1	0.593	1.986	6.946
Vibration 2	0.594	1.982	5.384
Vibration 3	0.597	1.971	4.329
Vibration 4	0.599	1.964	3.952
Vibration 5	0.607	1.938	3.196
Vibration 6	0.619	1.899	2.636
Vibration 7	0.624	1.885	2.49
Vibration 8	0.626	1.877	2.416
Vibration 9	0.636	1.846	2.171
Vibration 10	0.645	1.818	2.001
Vibration 11	0.668	1.748	1.669
Vibration 12	0.674	1.729	1.599
Vibration 13	0.676	1.723	1.578
Vibration 14	0.72	1.595	1.212
Vibration 15	0.745	1.526	1.064
Vibration 16	0.788	1.412	0.87
Vibration 17	0.794	1.399	0.85
Vibration 18	0.811	1.355	0.788
Vibration 19	0.834	1.299	0.716
Vibration 20	0.869	1.219	0.624
Vibration 21	0.896	1.16	0.563
Vibration 22	0.926	1.097	0.505
Vibration 23	0.968	1.012	0.43

Table 3

D. Electric Moment

The dipole moment in a molecule is an important property that is mainly used to study the intermolecular interactions involving the non-bonded type dipole–dipole interactions, because higher the dipole moment, stronger will be the intermolecular interactions. In the absence of experimental data, the values of polarizability and hyperpolarizability calculated at the same level of theory and the same basis set for the compound BMB, can provide a satisfactory comparison of these quantities.

Calculated dipole moment (μ, in Debye), mean polarizabilit ($\bar{\alpha}$, in a.u.), anisotropy of polarizability (Δα,in a.u.) and first hyperpolarizability (β, in a.u.) of BMB by DFT by B3LYP/6-31G(d,p).

Dipole moment		Polarizability		Hyperpolarizability	
μ_x	2.2399	α_{xx}	-115.0351	β_{xxx}	84.7803
μ_y	0.9507	α_{yy}	-85.1199	β_{yyy}	-27.0337
μ_z	0.4156	α_{zz}	-109.3771	β_{zzz}	5.1368
		α_{xy}	1.6480	β_{xyy}	-19.5231
		α_{xz}	-7.4247	β_{xxy}	30.2569
		α_{yz}	1.4067	β_{xxz}	14.5276
				β_{xzz}	18.5722
				β_{yzz}	-2.0060
				β_{yyz}	5.2307
				β_{xyz}	22.3774

The component of dipole moment μ, polarizability α and the first hyperpolarizability β can be calculated by using the following equations

$\mu = (\mu_x^2 + \mu_y^2 + \mu_z^2)^{1/2}$

$\bar{\alpha} = 1/3(\alpha_{xx} + \alpha_{yy} + \alpha_{zz})$

$\Delta\alpha = 1/\sqrt{2}\{[(\alpha_{xx} - \alpha_{yy})^2 + (\alpha_{yy} - \alpha_{zz})^2 + (\alpha_{zz} - \alpha_{xx})^2 + 6\alpha^2{}_{xz}]]\}^{1/2}$

First order polarizability $\beta = [(\beta_{xxx} + \beta_{xyy} + \beta_{xzz})^2 + (\beta_{yyy} + \beta_{xxy} + \beta_{yzz})^2 + (\beta_{zzz} + \beta_{xxz} + \beta_{yyz})^2]^{1/2}$

Using these equations values for the reported compound BMB comes out to be as follows....

$\mu = 2.4866$

$\bar{\alpha} = 103.1773$

$\Delta\alpha = 30.3817$

$\beta = 87.4535$

V. CONCLUSION

In the present work we have calculated the geometric parameters, the vibrational frequencies and NLO properties of 4-benzyloxy-3-methoxy-benzaldehy by using Becke-3Lee-Yang-Parr (B3LYP) functional supplemented with the standard 6-31G (DP) basis and compared these values with the experimentally recorded FTIR, IR (KBr and nuzol) and Raman spectra. In general, a good agreement between experimental and calculated normal modes of vibrations have been observed. We also calculated thermodynamic properties as heat capacity, entropy, enthalpy and Gibb's free energy of the titled compounds at different temperatures along with dipole moment, polarisability and hyperpolarisability .

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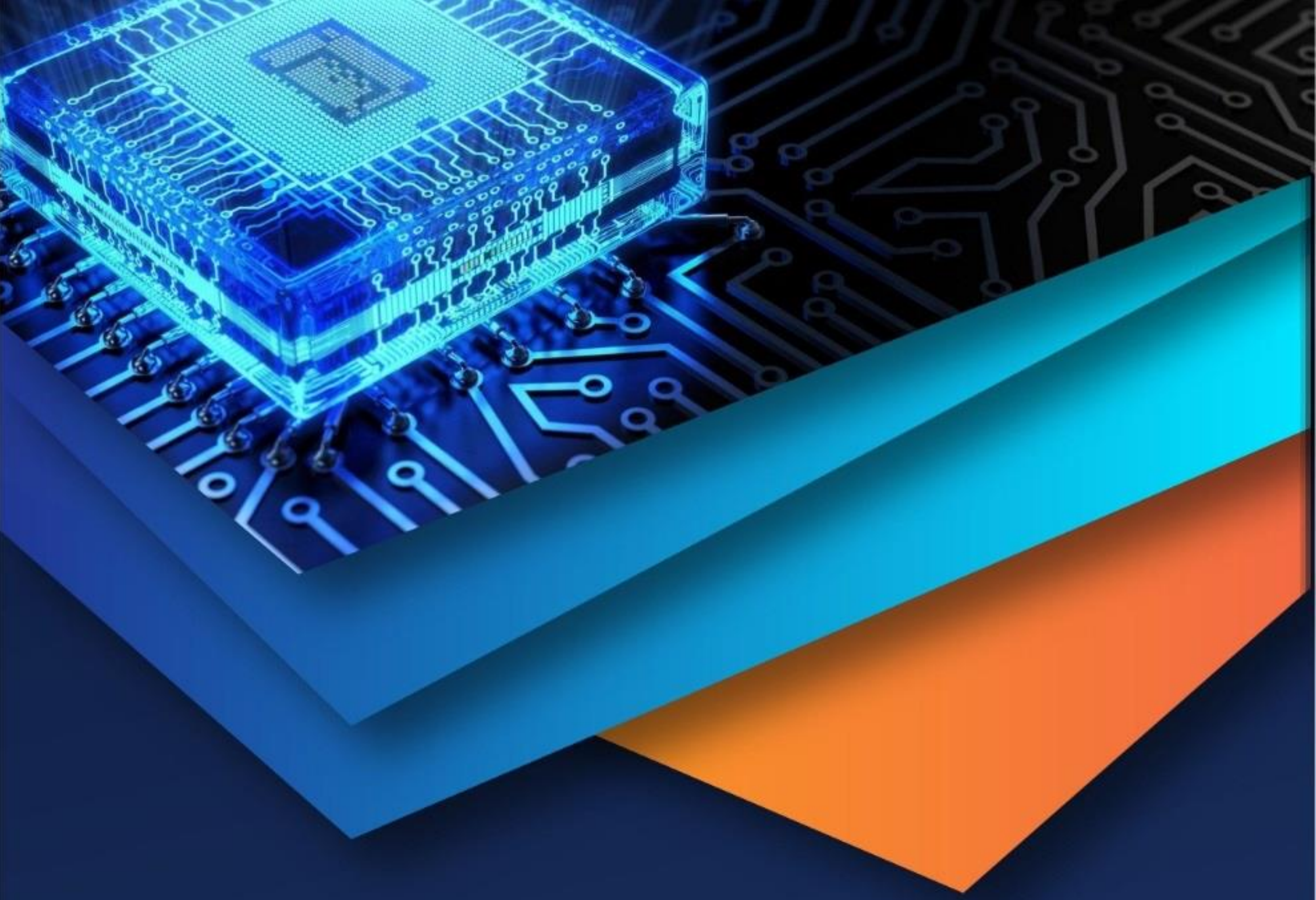

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