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Spectroscopic and Second Harmonic Generations Studies of 5-Bromo-2-methoxybenzonitrile by DFT

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ABSTRACT

Equilibrium geometric structure of 5-Bromo-2-methoxybenzonitrile (5B2MOBN) has been carried out through quantum mechanical calculations aided by Density Functional Theory (DFT). Geometrical parameters (bond length, bond angle and dihedral angle) are predicted by using DFT levels employing HF/B3LYP methods with 6-311++G (2d,p) as basis set. The FT-IR and FT-Raman spectra of the 5B2MOBN were recorded and analyzed by the same level of theory. Frequency doubling and Second Harmonic Generation (SHG) applications are exist in the title molecule, so that the Non Liner Optical (NLO) properties were calculated by the same method with different basis sets.

Keywords: 5B2MOBN, DFT, VEDA, TED

INTRODUCTION

Benzonitrile is the child molecule to the parent molecule ammonia to toluene, which had the enormous changing with the consequence of the particular ratio.[1] The fragrances, cosmetics, steroid, aromatic alcohols for color removers, solvents for fatty acids, hydrocarbons and oils are used with benzonitrile as a chemical broker. In recent researchers used Benzonitrile as most excellent solvent and versatile precursor chemical intermediate in many derivatives. Benzonitrile is a cyano group Benzonitrile is a colorless, almond-like odor salt, sharp taste[2] and boiling point at 190.7°C at 760 mm Hg[3]. Benzonitrile compounds had high toxic and irritating product. World Wide Organization set the range of benzonitrile while using the daily usage products. Toxicity effect used for evaluated in prokaryotic and eukaryotic systems. Which evaluation provided the sharp detail and carcinogenicity, chronic toxicity, and mutagenicity[4]. Anisole (methoxybenze) is another form of benzonitrile as it allows for dipolar and dispersion interactions while its capability to be involved in stronger interactions, such as hydrogen bonds, is limited to the role of proton acceptor.In analytical chemistry, the ortho- substituted derivatives of bromo are used as reagents also identified the anesthetic problems and brain diseases are cured through these drugs[5]. The benzene ring in 5-Bromo-2-methoxybenzonitrile (5B2MOBN) has three substituents such that the bromo and methoxy groups are at meta and ortho position respectively with respect to the cyano group. The methoxy and cyano groups are generally referred to as electron donating substituents in aromatic ring systems. The joining of cyano group in benzonitrile and the aromatic ring creates the migration of the nitrogen atom.

Associations of molecular structural design, nonlinear retort and hyperpolarizability were finding from the vibrational spectra studies of the molecules. The structure of the particle has been leaded by the spectra in juxtaposition through quantum chemical computations. For the spectral approaches unchangeable due to different theoretical methods and series of semi empirical to DFT approaches because every method had its inbuilt capacity[6]. To investigate the structural and vibrational characteristics were executed by HF level ab initio calculations. The present letter 5-Bromo-2-methoxybenzonitrile (5B2MOBN) have inspected both observed and calculations method. The literature review concluded that, there are no publications of the title compound 5B2MOBN using the theoretical methods. From the equilibrium molecular structure, parameters and vibrational assignments help to determine the results of the interior properties of the molecules. Hyperpolarizability and thermodynamical properties are predicted using the HF/DFT methods using the hybrid basis sets.

Experimental details

The compound 5B2MOBN provided a sturdy purity of larger than 99% and used as such without any additional refinement by Sigma-Aldrich Chemical Company, the USA. The FT-Raman (FTR) spectrum of 5B2MOBN has been recorded using 1064 nm line of Nd: YAG laser as excitation wavelength in the region 50-3500 cm^{-1} on a EZRaman, En wave optronics, USA IFS 66 V spectrometer. The Fourier transform infra-red (FTIR) spectrum was recorded using 8400S Bruker, Alpha T, and Germany infrared spectrophotometer using pellet technique in the region 4000–400 cm^{-1}. At the room temperature with scanning speed of 30 cm^{-1} min^{-1} the spectra are traced. The Fig.2 & Fig.3 shows the association of both observed and calculated IR and Raman spectra of 5B2MOBN. The above spectra are conceded out at the Department of Nanotechnology, Noorul Islam Centre for Higher Education (NICHE), kumaracoil, Thackalay, Kanyakumari District.

The spectra are computerized using the HF/B3LYP with basic set and the output spectra are monitored threw Gauss sum program, which gives the Raman intensities spectra directly[7]. This program equating the intensity theory of Raman scattering derived relationship and produces the modified Raman intensities data. The assignments give the same results while compared with the three basic sets. The Raman intensity data also merged with the dynamic basic sets which confirmed the formation of methylbenzonitrile. The calculated vibrational frequencies are tabulated as shown in Table. 3.

Computational details

The GAUSSIAN 09W program is used for predicted the quantum computational calculations of 5B2MOBN with the original version with three parameter functional by way of applying ab-initio Becke-Lee-Yang-Parr hybrid method in correlations HF/B3LYP[8] level with basis set on Intel Core i3 3.3GHz processor personal computer to derive the complete geometry optimization[9]. Gaussian software is a super positioning tool for developing fields of computational physics like structural analysis, reaction mechanisms, potential energy values, charge distributions and excitation energies of the compound[10]. The single point energy calculation is computing the energies of specific molecular structures and the allied molecular properties are predicted initially. Geometry optimizations calculating equilibrium structure of molecules, optimizing transition structures and energy minimizations at dynamic basic sets. From the second derivatives the energy has been calculated the FT-IR, Raman frequency computing and intensities plots are done by the Gauss sum program. The vibrational assignments with TED are calculated and explained using the Scaled quantum mechanical program using VEDA 4.0. Software[11]. An elevated degree of precision at the customarily considerations along with obtainable linked by the GAUSSVIEW program are made by the molecules vibrational frequency assignments.

RESULTS AND DISCUSSION

Optimized geometry

5B2MOBN compound optimized structure has been illustrated (Fig.1). The stable minimum energy calculated as -3008.21301245 and -3012.6812156 a.u, by HF and B3LYP functional with the standard basis sets. The predicted atomic lengths, atomic angles and torsion angle or dihedral angles from the above method are tabulated in Table.1. There is no data on the optimized structure and equilibrium parameters of 5B2MOBN do not exist in earlier reports through the literature survey. The microwave data are slightly small while compare with theoretical value of the optimized atomic lengths be in the right places to isolated title compound in gaseous phase. The predicted geometrical parameters of the two different basis sets are almost similar. The theoretical values had good agreement with the microwave data. Benzene ring had six carbon atoms and hydrogen atoms which carbons atoms had same lengths and angles and hydrogen atoms had some changes. The molecule have modify in the different chemical and physical assets because of the hydrogen in benzene ring which acts as the trepidation of the valence electron distribution. The recent molecule interactions to the substituents are indicating the benzene ring angular changes[12].

The molecule has seven carbons bonds, six C–H, two C-O, C–N and C-Br bonds. There is no crystal structure for the 5B2MOBN, benzene ring appears a small hazy with carbon to carbon atom bond length next to the substitutions place (≈1.40Å) longer than the carbon bond (C5-6) in the middle of the ring substituted in the bromo (≈1.36Å). The distorted elucidates that the substituted on the ring can affect the hybridization and bond lengths of the carbon atoms. The bond length of C-C increase while compare with benzene ring this shows the angle between substituted atoms has little modified hexagonal structure of the angles. From that result, it is found that the benzene ring has almost the same length of the all carbons bond and deviation should be around 0.005 Å it only corresponds with the earlier reports. The length of the Ca≡N bond had 1.15Å is computed by both basic sets and 1.13 Å is observed for the benzonitrile in early results. Both results had good correlation and the minimum deviation level is 0.02Å, whose result is shorter than the single bond carbon and bromo group as valued is 1.13 Å for both the basis sets. At last, the length of the carbon bromo bond is calculated and merged with the observed value as 1.88 Å which is reported by M. Elanthiraiyan *et al.,* 13. The angles between the bonds have been predicted by an atom that has the corresponding results while comparing with the microwave data.

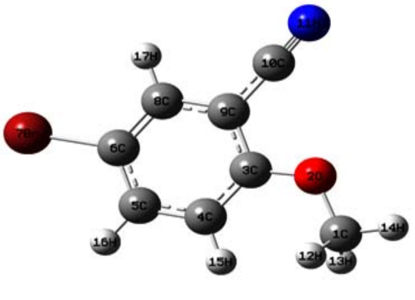

Fig.1. Optimized structure of 5B2MOBN

Vibrational spectra

There are 45 vibrational assignments are assigns for the 5B2MOBN molecule. In the 45 assignments C1 point group symmetry. Every vibration intended for N atomic molecules had 2N-3 and N-3 is both bending. As a result 14 in-planes (β) and 9 out of plane (δ) bending are identified for 5B2MOBN 28 of all 45 vibrations.

In the novel compound of 5B2MOBN are premeditated the harmonic vibrational frequencies at B3LYP level by various basis sets have specified in Table.2. Experimental data and the portrayals alarming the mission also have designated in Table 2 gives the coherent basis for the assignments and shows that the molecules assignments as well as IR & Raman intensities of the title molecule. In Figs.2 and 3 shows the comparisons of experimental and calculated spectra.

CH vibrations

Four kinds of CH moieties are calculated in the title compound 5B2MOBN. In this CH moieties have been listed, six CH stretching, in plane as well as torsion vibrations. The scenery of the substituent does not align because of these stretching vibrations. The stretching has most feasible frequency between the regions at

3100-3000cm^{-1} [14]. The calculated stretching vibrations of the title compound region, in between 3202-3005cm^{-1}. There is no experimental frequencies have been observed. The calculated CH in-plane bending vibrations of 5B2MOBN occurs in the region of 1600-1100 cm^{-1} and observed FTIR and FTR spectra at 1532, 1517, 1480, 1429, 1250, 1175, 1125cm^{-1} and 1482, 1312, 1214 cm^{-1}, respectively. The CH out-of-plane bending occurs at the region 950-800cm^{-1} generally. The calculated out-of-plane bending vibrations of 5B2MOBN are found at 952, 920, 822, cm^{-1}. Observed FTIR and FTR spectraoccurred in the region 876 and 908 cm^{-1} correspondingly. In this case, the in-plane and out-of-plane bending has been merged with the torsion vibrations. Calculate and observed values good agreement with each other.

CBr vibrations

CBr moieties have been tabulated on the basis of calculated energy distribution and separated three kinds of modes. Six stretching and in-plane bending vibrations are packed in the CBr atom. The CBr stretching and bending vibrations are incorporate with each other. In the literature survey, the authors assigned vibrations frequency

Table.1: Equilibrium parameters of 5B2MOBN

Bond Length(Å)	HF	B3LYP	Exp	Bond Angle(°)	HF	B3LYP	Dihedral Angle(°)	HF	B3LYP
C1-O2	1.43	1.43	1.44	O2-C1-H12	109	109	C9-C10-N11-H14-1	180	180
C1-H12	1.07	1.07	0.98	O2-C1-H13	109	109	C9-C10-N11-H14-2	180	180
C1-H13	1.07	1.07	0.95	O2-C1-H14	109	109	H12-C1-O2-C3	-90	-60
C1-H14	1.07	1.07	0.95	H12-C1-H13	109	109	H13-C1-O2-C3	30	60
O2-C3	1.3	1.43	1.37	H12-C1-H14	109	109	H14-C1-O2-C3	150	180
C3-C4	1.4	1.4	1.402	H13-C1-H14	109	109	C1-O2-C3-C4	0	-30
C3-C9	1.4	1.4	0.95	C1-O2-C3	120	109	C1-O2-C3-C9	180	150
C4-C5	1.36	1.4	1.438	O2-C3-C4	120	120	O2-C3-C4-C5	180	180
C4-H15	1.07	1.07	0.95	O2-C3-C9	120	120	O2-C3-C4-H15	0	0
C5-C6	1.36	1.4	1.384	C4-C3-C9	119	120	C9-C3-C4-C5	0	0
C5-H16	1.07	1.07	0.95	C3-C4-C5	120	120	C9-C3-C4-H15	-180	-180
C6-Br7	1.91	1.91	1.88	C3-C4-H15	120	120	O2-C3-C9-C8	-180	180
C6-C8	1.36	1.4	1.38	C5-C4-H15	120	120	O2-C3-C9-C10	0	0
C8-C9	1.4	1.4	1.38	C4-C5-C6	121	120	C4-C3-C9-C8	0	0
C8-H17	1.07	1.07	0.95	C4-C5-H16	120	120	C4-C3-C9-C10	180	180
C9-C10	1.4	1.4	1.4	C6-C5-H16	120	120	C3-C4-C5-C6	0	0
C10-N11	1.15	1.15	1.13	C5-C6-Br7	120	120	C3-C4-C5-H16	180	180
				C5-C6-C8	121	120	H15-C4-C5-C6	180	180
				Br7-C6-C8	120	120	H15-C4-C5-H16	0	0
				C6-C8-C9	120	120	C4-C5-C6-Br7	-180	-180
				C6-C8-H17	120	120	C4-C5-C6-C8	0	0
				C9-C8-H17	120	120	H16-C5-C6-Br7	0	0
				C3-C9-C8	119	120	H16-C5-C6-C8	-180	180
				C3-C9-C10	120	120	C5-C6-C8-C9	0	0
				C8-C9-C10	120	120	C5-C6-C8-H17	180	180
							Br7-C6-C8-C9	-180	180
							Br7-C6-C8-H17	0	0
							C6-C8-C9-C3	0	0
							C6-C8-C9-C10	-180	-180
							H17-C8-C9-C3	-180	180
							H17-C8-C9-C10	0	0

range of 1129–480 cm^{-1} while the Carbon interactions with others heavy atoms like Cl, Br, I [15]. The 5B2MOBN compound has the strong both vibrations in the region of 876, 665 and 310, 258, 126 cm^{-1} found from IR and Raman spectrum, respectively. Torsion vibrations calculated frequency of the title molecule transpire in the range at 319, 223, 116 cm^{-1}. These vibrations are very well agreed with literature survey.

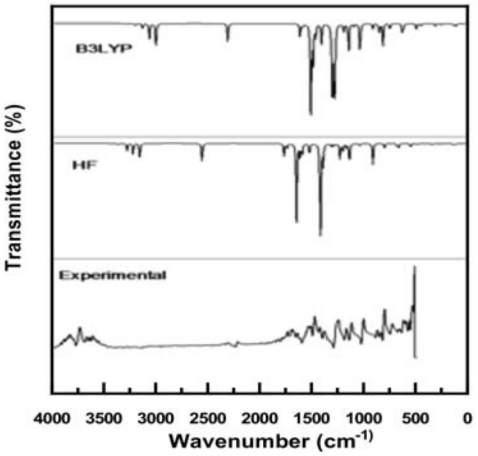

Fig.2. Experimental and theoretical DFT/B3LYP FT-IR of 5B2MOBN

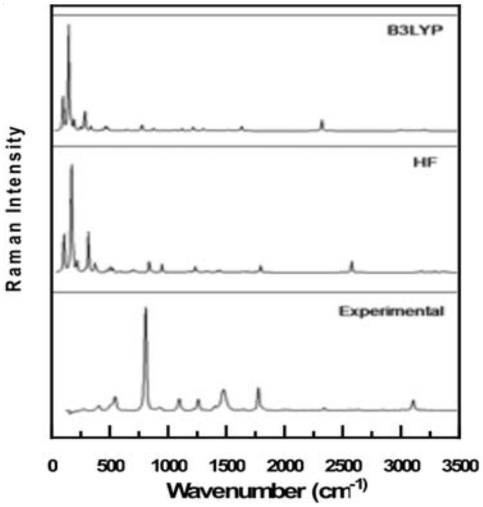

Fig.3. Experimental and theoretical DFT/B3LYP FTR of 5B2MOBN

Ca≡N vibrations

In the CN moieties, stretching frequency is the intensively localized one due to the TED for this frequency contains good contribution from that constant value of stretching force. In the benzonitrile molecule, the cyano group (Ca≡N) vibrational wave number is almost unchanged because of it joined together the phenyl ring as a new substituent. For the aromatic compound which bears a Ca≡N group attached to the ring, a band of good intensity has been absorbed in the region 2240–2221 cm^{-1} [16] and it is being attributes to Ca≡N stretching. Br is the electron acceptor groups; it decrease the IR band intensity and increases the wave number value to the higher limit of the characteristic spectral region. CH_3 is the electrons donating groups, it increase IR intensity and decrease wave number value[17]. These electron acceptor groups are the main impact for the shifting for Ca≡N vibrational wave number. FTR spectra frequency at 2338 cm^{-1} for Ca≡N (ν) vibrations found for 5B2MOBN. The calculated wavenumbers of stretching vibrations at 2313cm^{-1} coincide with the FTIR value. This is the ideal frequency of the whole molecule which confirmed the CN stretching with 90% assignment. The bending vibrations(β) of the molecule for Raman and FTIR spectra spotted at 424, 310, 126 cm^{-1} and 665, 626 cm^{-1}, respectively[18]. These experiment values are well agreement with the calculated frequencies.

C-C and C-C-C vibrations

Benzonitriles are the substituents cyanogens groups and the benzene ring has almost the same length of the all carbons bond and minimum deviation. The thirteen stretching (mode no. 13, 14, 20, 22, 27, 30, 31, 32, 33, 34, 39, 40, 41) carbon vibrations slouch in the region 500-1850 cm^{-1} and ten bending of vibrations slouch above the region 1300 cm^{-1} [19]. From the research, the six similar carbon bonding can produce benzene the same time that ring vibrating the seven C-C stretching modes are scanned through FTIR in the region at 1646, 1532, 1429, 1387, 1250, 1125, 876 cm^{-1} and the five FTR at 2338, 1644, 1312, 1214, 424 cm^{-1} coincides each other. The recorded spectral values of C-C-C bending modes at 1010, 876, 665, 626 and 1030, 126 cm^{-1} values are equal with predicted numerical.

CCCC torsional vibrations:

The ring torsions have been assigned in the region at below 800 cm^{-1} which is discussed in present paper referred by earlier reports[20]. The IR and Raman spectra peak observe in the region at 734, 601, 520 and 714, 604, 490 cm^{-1} respectively. These peaks have been calculated at the region at 751, 595, 501, 402, 146, 116 cm^{-1} by B3LYP methods which are well merge with observed values. And these wavenumbers are mixed with CCCN torsions in the investigated molecules.

Table.2: The observed (FT-IR, FT-Raman) and calculated frequencies (cm-1), IR intensity (km mol-1), Raman intensity (Å4 amu-1) and probable assignments of 5B2MOBN

		Experimental (cm^{-1})		Wavenumbers(cm^{-1}) B3LYP/6-311++G(2d,p)					
Normal Modes	Symmetry spices	FT-IR	FT-Raman	Scaled	Un Scaled	IR Intensity (Km/mol)	Raman Intensity	Force Constant	Vibrational assignments
1	A			73	73	0.38	6115.73	0.012	
2	A			116	116	0.391	479.236	0.037	τCOCC(46)+τCCCC(44)+τCCCBr(10)
3	A		126	121	121	4.194	18172.2	0.109	βCCC(45)+βCCN(34)+βCCBr(11)
4	A			140	141	4.007	1618.19	0.064	τCCCC(29)+τCOCC(23)+τCCCBr(22)+τCCCN(11)
5	A			169	169	1.289	1692.51	0.082	βCCBr(39)+βCCO(32)+βCOC(15)
6	A			223	224	0.002	650.28	0.034	τHCOC(81)
7	A		258	260	261	3.097	4559.91	0.354	νBrC(39)+βCCBr(15)+βCOC(13)
8	A		310	312	313	0.663	704.86	0.3	βCCBr(20)+βCOC(20)+νBrC(16)+βCCO(14)+βCCN(11)
9	A			319	320	3.995	284.242	0.375	τCCCO(36)+τCCCBr(29)+τHCOC(12)+τCCCN(10)
10	A			402	404	0.309	299.429	0.402	τCCCC(64)+τCCCN(22)
11	A		424	437	438	0.079	877.859	0.646	βCOC(33)+βNCC(17)+νCC(13)
12	A			458	460	4.738	812.124	1.217	βCCC(46)+νCC(18)
13	A	520	490	501	503	10.545	132.538	0.497	τCCCC(27)+τHCCO(26)+τHCCC(24)
14	A	601	604	595	597	0.688	118.217	1.114	τCCCC(64)+τCCCN(24)
15	A	626		625	627	7.61	302.928	1.246	βCCO(20)+βCCN(11)+βCCC(11)
16	A	665		637	639	15.356	112.265	1.969	βCCC(54)+νBrC(12)+βCCN(10)
17	A	734	714	751	754	0.007	34.966	0.988	τCCCC(89)
18	A			755	758	11.129	1474.36	1.854	νCC(54)+νOC(15)
19	A	843		822	825	34.914	10.359	0.674	τHCCO(61)+δCCCH(26)
20	A	876		858	861	19.842	637.087	3.249	βCCC(29)+νCC(17)+νBrC(13)
21	A		908	920	924	9.609	9.572	0.742	δCCCH(86)
22	A			952	956	0.189	1.742	0.727	δCCCH(61)+τHCCO(24)
23	A	1010	1030	1043	1047	52.939	259.105	5.189	νOC(60)+βCCC(13)
24	A			1100	1104	4.963	445.954	1.504	νOC(47)+βHCC(16)
25	A	1125		1152	1156	48.912	95.63	1.806	βHCC(24)+νCC(12)
26	A	1175		1166	1171	0.908	46.612	1.025	βHCO(70)+δCHOH(19)
27	A			1197	1202	7.67	292.999	1.595	δCHOH(35)
28	A		1214	1202	1207	8.119	654.267	1.34	δCHOH(33)+βHCC(12)+νCC(11)
29	A	1250		1284	1289	98.393	416.181	2.063	βHCC(38)+νOC(20)+νCC(15)
30	A			1295	1300	86.941	160.095	2.717	νCC(26)+βHCC(20)+νOC(15)
31	A	1387	1312	1312	1316	114.304	118.08	3.923	νCC(41)+νOC(11)

32	A	1429		1415	1420	32.986	57.402	4.2	νCC(52)+βHCC(22)
33	A	1480	1482	1470	1476	20.697	24.221	1.607	βHCH(25)+δCHOH(22)+βHCO(14)+βHCC(13)
34	A			1491	1497	10.233	161.646	1.38	βHCH(50)+δCHOH(36)
35	A			1495	1500	54.631	46.681	1.419	βHCH(80)+δCHOH(12)
36	A	1517		1515	1521	159.324	229.074	3.128	βHCC(36)
37	A	1532		1594	1599	6.602	204.821	10.247	νCC(62)+βHCC(11)
38	A	1646	1644	1619	1625	23.29	975.256	9.354	νCC(61)
39	A		2338	2313	2323	32.597	2213.49	40.311	νNC(90)+νCC(11)
40	A			3005	3017	46.786	371.785	5.546	νCH(91)
41	A			3067	3080	26.113	116.481	6.187	νCH(99)
42	A			3133	3146	10.734	202.811	6.415	νCH(90)
43	A			3183	3196	0.569	91.433	6.558	νCH(100)
44	A			3197	3211	0.439	56.729	6.634	νCH(98)
45	A			3202	3216	2.891	235.623	6.655	νCH(98)

ν-stretching; β-in plane bending; δ-Out-of-plane bending; τ-torsion; TED-Total Energy Distribution

C-O vibrations

The observed region 1360–1260 cm^{-1} is the best frequency vibration for carbonyl group[21]. For the reason that of its sky-scraping intensity[22] and the comparatively interference-free province in which it occurs, this band is logically effortless to distinguish. Vijay Rastogi *et al.,* assigned vibrations of C-O band observed at 1348 cm^{-1} (DFT) as the stretching mode. M. Suhasini *et al.,* assigned stretching vibrations of C-O band observed at 1646, 1629 cm^{-1} in the FTIR spectrum and 1633 in Raman spectrum. In the current vocation, the bands observed in 1387, 1250,1010 cm^{-1} at the infrared and 1312, 1030 cm^{-1} in Raman spectrum are assigned to the C=O stretching mode of vibrations. The hypothetically pragmatic frequencies are in very good agreement with the experimental frequencies. These C=O vibrations are also shown fairly good coherent in literature survey. The 2-(4-bromophenyl)-2-oxoethyl-3-methylbenzoate has observed at1385 cm^{-1} in (C-O) stretching mode[23]. For the title compound, has assigned the stretching at 1387 cm^{-1} (DFT) and 1312 cm-1 (Raman).

Optical property

The hyperpolarizability is contributed by the structure, bonding and vibrational of the molecule. The dipole moment (μ) and hyperpolarizability of the benzonitrile is high. In the recent molecule has been calculated the enhanced hyperpolarizability value which is due to the substituent of the benzonitrile. The bond and vibrational results are confirmed the envelope to the hyperpolarizability enlargement of the 5B2MOBN molecule. In the fields such as telephoning, signal transferring and fiber optic cables, NLO enhance the functions for the developing technologies like frequency modulation, optical changing, optical controlling and optical logical circuits[24]. The first hyperpolarizability (β) polarizability (α) and anisotropy of polarizability[25] (Δα) of 5B2MOBN is calculated using DFT with the above basic set and can be evaluated using equations (1) (2) (3) respectively. The Table.3 listed the numerical values of above mentioned parameters. The electric is the task for the energy of the scheme because an electrical meadow exists in the molecule. 3 3 3 matrix is used for determined the hyperpolarizability. Kleinman symmetry diminished the 27 mechanisms into 10 mechanisms[26].

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

$$\alpha = \frac{1}{3}(\alpha_{xx} + \alpha_{yy} + \alpha_{zz}) \quad (2)$$

$$\Delta\alpha = \frac{1}{\sqrt{2}}\left[(\alpha_{\chi\chi}-\alpha_{yy})^2 + (\alpha_{\chi\chi}-\alpha_{zz})^2 + (\alpha_{zz}-\alpha_{\chi\chi})^2 + 6\alpha^2_{\chi z}+6\alpha^2_{\chi y}+6\alpha^2_{yz}\right]^{1/2} \quad (3)$$

$$\beta = [(\beta_{\chi\chi\chi}+\beta_{\chi yy}+\beta_{\chi zz})^2+(\beta_{yyy}+\beta_{zzy}+\beta_{y\chi\chi})^2+(\beta_{zzz}+\beta_{z\chi\chi}+\beta_{zyy})^2]^{1/2} \quad (4)$$

The calculated values of α and β are 2587.1041×10^{-33}esu and1767.4709×10^{-33} esu. Ideal molecule urea is used for determined the comparative purpose. The compound has the values 2.151D and 1.7674×10^{-33} esu of μ and β respectively. The μ of compound is approximately 1.56 times greater than that of urea and the β of compound is 4.74 times greater than that of urea (μ and β of urea are 1.3732 Debye and 0.3728 ×10^{-30}esu with the same method). The recent molecule has steady state potential for NLO applications like frequency doubling and communications that is confirmed by the recent research[27].

Table.3: Optical properties of 5B2MOBN

Parameters	B3LYP/6-311++G(2d,p)	B3LYP/6-311++G(d,p)	Parameters	B3LYP/6-311++G(2d,p)	B3LYP/6-311++G(d,p)
μ_x	0.5231839	0.5425969	β_{xxx}	150.575	106.644
μ_y	-0.8954072	-0.907651	β_{xxy}	15.7744	21.0226
μ_z	-1.8846654	-1.8997386	β_{xyy}	30.2549	25.8986
μ	2.1511Debye	2.1742Debye	β_{yyy}	-83.021	-85.125
α_{xx}	169.9052472	166.3009652	β_{xxz}	57.1005	43.6984
α_{xy}	-21.2152338	-21.6155069	β_{xyz}	-45.732	-46.307
α_{yy}	86.3503433	82.8495989	β_{yyz}	-12.325	-15.073
α_{xz}	12.4692927	11.681339	β_{xzz}	17.2665	7.27064
α_{yz}	19.3370896	19.6332495	β_{yzz}	16.661	18.7448
α_{zz}	129.6060502	126.0585381	β_{zzz}	-37.437	-47.344
α_0	299.4576x10^{-33}esu	144.5724x10^{-33}esu	β_0	1767.4709x10^{-33}esu	1280.1140x10^{-33}esu
α	2587.1041x10^{-33}esu	291.1700x10^{-33}esu			

CONCLUSION

From the HF/DFT methods by 6-311++G (2d, p) basis sets, computed the geometrical parameters and optimized structure. The research the experimental FT-IR, FTR spectroscopic studies are investigated first time and explained vibrations assignments with TED% using the B3LYP method. The theoretical spectra are predicted using computational methods and well agreement with experimental results. The μ and β values of the compound were 1.56 and 4.74 times greater than that of urea, respectively.These properties show that the title compound 5B2MOBN had good chemical stability, bioactivity and optics applications for helping the future researchers and innovative thinkers.

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