



Theoretical Spectroscopic and Second Harmonic Generations Studies of 5-Fluoro-2-Methyl Benzonitrile

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ABSTRACT

5-fluoro-2-methylbenzonitrile (5F2MLBN), a novel molecule has been reported after mutually experimental and theoretical approaches on molecular atomic structure, vibrational spectra, non-linear optics (NLO) properties. The FT-IR (400–4000 cm^{-1}) and FT-Raman spectra (50-3500 cm^{-1}) of 5F2MLBN were recorded. The density functional HF methods with three higher basis sets were determined the molecular geometry, harmonic vibrational frequencies and bonding features of 5F2MLBN in the ground state. Finally, spectra of the title compound have good complement while compared with the calculation results were applied to simulate infrared and Raman spectra.

Keywords: 5F2MLBN, 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 ratio¹. 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 taste² and boiling point at 190.7°C at 760 mm Hg³. 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 mutagenicity⁴. Anisole (methylbenze) 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 fluoro are used as reagents also identified the anesthetic problems and brain diseases are cured through these drugs⁵.

Benzoic acid reacts with lead thiocyanates, Benzonitrile phenyl cyanic compound will produced by heating⁶. The pH level of the food will thaw out the effectiveness of benzoic acid. Acidic food, beverages, pickles and acidified foods are preserved with benzoic acid. In the field of medicine, these acid has used as an antibacterial and excellent painkiller in the near the beginning of 20th century⁷. Benzoic acids used for the production of Whitefield's ointment, tincture and Friar's balsam⁸.

The benzene ring in 5-Fluoro-2-Methyl Benzonitrile (5F2MLBN) has three substituents such that the fluoro and methyl groups are at meta and ortho position respectively with respect to the cyano group. The methyl 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 capacity⁹. The DFT has been accepted as a popular post-HF approach for the computation of molecular structure, vibrational frequencies and energies of molecule by the ab initio quantum chemistry community¹⁰. The present letter 5-Fluoro-2-Methyl Benzonitrile(5F2MLBN) have inspected both observed and calculations method. The literature review concluded that, there are no publications of the title compound 5F2MLBN 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 parameters are predicted using the DFT methods using the hybrid basis sets.

Experimental details

The spectroscopic analytical purpose, The Fourier-transform infrared (FTIR) and The Fourier-transform Raman (FT Raman) spectra have been recorded at normal temperature in the region 400-4000 cm^{-1} and 50-3500 cm^{-1} respectively. Infrared spectrum recorded using 8400S Bruker, Alpha T, and Germany infrared spectrophotometer with scanning speed of 30 $\text{cm}^{-1} \text{min}^{-1}$ the spectra are traced. FT Raman spectrum has been recorded using 1064 nm line of Nd:YAG laser as excitation wavelength on an EZRaman, Enwaveoptronics, and USA IFS 66 V spectrometer. All spectra recorded out at our campus of the Nanotechnology Department. The spectra are exposed in Figure. 2 & 3.

Computational details

The Gaussian 09W software package has been used for predicting the whole vibrational assignments and optimized geometrical parameters of 5F2MLBN with the original version¹¹. The complete geometry parameter has been derived from Becke-Lee-Yang-Parr hybrid (B3LYP) is the three parameter functional by way of applying ab-initio B3LYP hybrid method¹² on Intel Core i3 3.3GHz processor personal computer. The vibrational wavenumbers corrected by introducing the scaling factor. The Scaling factor values are 0.9556 and 0.9959 at (d,p) and cc-pvdz respectively¹³. The total energy distribution (TED) was calculated and explained using the Scaled quantum mechanical program using VEDA .4.0. Software¹⁴ and vibrational modes also calculated through their TED. 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. From the second derivatives of the energy has calculated the FT-IR, Raman frequencies are computing and intensities plots are done by the Gauss sum program¹⁵. The non-linear optical (NLO) assets such as dipole moment (μ), polarizability (α), anisotropy of polarizability (α_0), and first hyperpolarizability (β_0) calculated to understand the frequency doubling the SHG behavior of 5F2MLBN are computed and Thermo dynamical parameters are resolute by Gaussian 09 DFT.

RESULTS AND DISCUSSION

Molecular Geometry Optimizations

5F2MLBN compound optimized structure has been illustrated (Fig. 1). The stable minimum energy calculated by B3LYP functional with the standard three basis sets (Table 2.1). The predicted atomic lengths, atomic angles and torsion angle or dihedral angles from the above method are tabulated in Table. 2. There is no data on the optimized structure and equilibrium parameters of 5F2MLBN 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 changes¹⁶.

The molecule has seven carbons bonds, eight C-C, six C-H, one C-N and C-F bonds. There is no crystal structure for the 5F2MLBN, benzene ring appears a small hazy with carbon to carbon atom bond length next to the substitutions place ($\sim 1.40\text{\AA}$) longer than the carbon bond (C2-F9) in the middle of the ring substituted in the fluoro ($\approx 1.35\text{\AA}$). 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\AA it only corresponds with the earlier reports. The length of the C \equiv N bond had 1.15\AA is computed by all basic sets and 1.15\AA is observed for the benzonitrile in early results. All results had good correlation and the minimum deviation level

is 0.02\AA , whose result is shorter than the single bond carbon and fluoro group as valued is 1.35\AA for three basis sets. At last, the length of the carbon fluoro bond is calculated and merged with the observed value¹⁷. The angles between the bonds have been predicted by an atom that has the corresponding results while comparing with the microwave data.

Table.1: Universal minimizations energy of 5F2MLBN

Basic sets	Energy(a.u)
B3LYP/6-311++G(d,p) (A)	-463.1727458
B3LYP/cc-pvdz (B)	-463.1727459
B3LYP/Aug-cc-pvdz (C)	-463.0990167

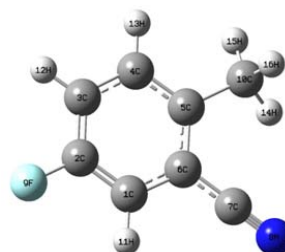


Fig.1. Optimized structure of 5F2MLBN

Vibrational spectra

There are 42 vibrational assignments are assigns for the 5F2MLBN molecule. In the 42 assignments C1 point group symmetry. Every vibration intended for N atomic molecules had $2N-3$ and $N-3$ is both bending. As a result 29 in-planes (β) and 13 out of plane (δ) bending are identified for 5F2MLBN 28 of all 42 vibrations.

In the novel compound of 5F2MLBN are premeditated the harmonic vibrational frequencies at B3LYP level by various basis sets have specified. Experimental data and the portrayals alarming the mission also have designated in Table.3 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 5F2MLBN. In this CH moieties have been listed, six CH stretching, in plane as well as torsion

Table. 2: Equilibrium parameters of 5F2MLBN

Bond Length(Å)	A	B	C	M.D	Dihedral Angle(°)	A	B	C
C1-C2	1.36	1.36	1.4	1.4	C6-C1-C2-C3	0	0	-0.003
C1-C6	1.54	1.54	1.4	1.4	C6-C1-C2-F9	180	180	-180
C1-H11	1.07	1.07	1.07		H11-C1-C2-C3	180	180	180
C2-C3	1.54	1.54	1.4	1.39	H11-C1-C2-F9	0	0	0.0005
C2-F9	1.35	1.35	1.35	1.35[18]	C2-C1-C6-C5	0	0	-0.008
C3-C4	1.36	1.36	1.4	1.39	C2-C1-C6-C7	180	180	180
C3-H12	1.07	1.07	1.07		H11-C1-C6-C5	180	180	180
C4-C5	1.54	1.54	1.4	1.39	H11-C1-C6-C7	0	0	-0.0076
C4-H13	1.07	1.07	1.07		C1-C2-C3-C4	0	0	0.004
C5-C6	1.36	1.36	1.4	1.39	C1-C2-C3-H12	180	180	-180
C5-C10	1.54	1.54	1.54		F9-C2-C3-C4	180	180	180
C6-C7	1.54	1.54	1.4		F9-C2-C3-H12	0	0	0.002
C7-N8	1.15	1.15	1.15	1.15	C2-C3-C4-C5	0	0	0.0055
C10-H14	1.07	1.07	1.07		C2-C3-C4-H13	180	180	-180
C10-H15	1.07	1.07	1.07		H12-C3-C4-C5	180	180	-180
C10-H16	1.07	1.07	1.07		H12-C3-C4-H13	0	0	0.004
Bond Angle(°)					C3-C4-C5-C6	0	0	-0.02
C2-C1-C6	120	120	120		C3-C4-C5-C10	180	180	180
C2-C1-H11	120	120	120		H13-C4-C5-C6	180	180	180
C6-C1-H11	120	120	120		H13-C4-C5-C10	0	0	-0.02
C1-C2-C3	120	120	120	122.8[18]	C4-C5-C6-C1	0	0	0.02
C1-C2-F9	120	120	120	118.7[18]	C4-C5-C6-C7	180	180	-180
C3-C2-F9	120	120	120	118.5[18]	C10-C5-C6-C1	180	180	-180
C2-C3-C4	120	120	120	119.9	C10-C5-C6-C7	0	0	0.02
C2-C3-H12	120	120	120		C4-C5-C10-H14	-150	-150	-90
C4-C3-H12	120	120	120		C4-C5-C10-H15	-30	-30	30
C3-C4-C5	120	120	120	120.2	C4-C5-C10-H16	90	90	150
C3-C4-H13	120	120	120		C6-C5-C10-H14	30	30	90
C5-C4-H13	120	120	120		C6-C5-C10-H15	150	150	-150
C4-C5-C6	120	120	120	120.1	C6-C5-C10-H16	-90	-90	-30
C4-C5-C10	120	120	120					
C6-C5-C10	120	120	120					
C1-C6-C5	120	120	120	120.2				
C1-C6-C7	120	120	120					
C5-C6-C7	120	120	120					
C5-C10-H14	110	110	109					
C5-C10-H15	110	110	109					
C5-C10-H16	110	110	109					
H14-C10-H15	110	110	109					
H14-C10-H16	110	110	109					
H15-C10-H16	110	110	109					

A- B3LYP/6-311++G(d,p)

B- B3LYP/cc-pvdz

C- B3LYP/Aug-cc-pvdz

M.D - Microwave Data (benzonitrile)

Table. 3 : 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 5F2MLBN

Normal Modes		Experimental (cm ⁻¹)		Scaled Wavenumbers (cm ⁻¹)			Raman Activity	Assignments with TED (%)
Mode	Label	FT-IR	FT-Raman	A	B	IR Intensity (Km/mol)		
1	A			79	80	0.13	0.4102	
2	A			130	130	0.21	0.7025	τCCCC(69)+τCCCN(12)
3	A		144	143	143	0.23	3.9458	βCCC(48)+βCCN(44)
4	A			154	154	0.25	0.2942	τCCCC(51)+τCCCF(27)
5	A			304	304	0.48	0.426	βCCC(53)+βCCF(20)
6	A		330	337	337	0.54	2.0035	τCCCF(45)+τCCCC(37)
7	A			403	403	0.64	1.4563	τCCCC(48)+τCCCN(34)
8	A			415	415	0.66	0.5394	βCCF(53)+βCCN(15) +βCCC(13)
9	A		434	446	446	0.71	5.7741	βCCC(58)+νCC(10)
10	A		484	492	492	0.78	0.474	τCCCC(67)+τCCCN(18)
11	A	531		498	498	0.79	9.3586	νCC(30)+βCCC(27)+νFC(10)
12	A	578		602	602	0.96	1.2148	βCCC(34)+βCCN(30)
13	A	666		627	627	1	1.9935	τCCCC(60)+τCCCN(17) +τCCCF(15)
14	A	701	708	720	720	1.15	0.3561	τCCCC(78)
15	A			723	723	1.15	7.6416	βCCC(46)+νCC(15) +νFC(10)
16	A	750	758	764	764	1.22	16.5348	βCCC(39)+νCC(28)
17	A	819		838	837	1.33	0.0978	τHCCF(50)+δCCCH(37)
18	A	887		898	898	1.43	0.0739	δCCCH(91)
19	A	937	944	955	955	1.52	14.6849	νCC(22)+νFC(18)+ βCCC(14)
20	A			965	965	1.54	0.072	δCCCH(49)+τHCCF(40)
21	A			1020	1020	1.63	2.5262	βHCC(29)+δCHCH(28) +νCC(11)
22	A	1081		1062	1062	1.69	0.134	βHCC(58)+δCHCH(28)
23	A			1117	1117	1.78	2.1453	βHCC(25)+νCC(14) +βCCC(11)
24	A	1142		1170	1170	1.86	1.8219	βHCC(56)+νCC(20)
25	A			1209	1209	1.93	6.4833	νCC(40)+βHCC(25)
26	A	1247	1278	1272	1272	2.03	60.2073	νFC(21)+νCC(10)
27	A			1292	1291	2.06	2.5717	βHCC(54)
28	A	1390		1325	1325	2.11	6.1959	νCC(56)
29	A			1423	1423	2.27	11.9581	βHCH(49)+βHCC(26) +δCHCH(22)
30	A	1459		1434	1434	2.29	2.551	νCC(39)+βHCC(13)
31	A			1484	1484	2.36	8.6356	δCHCH(65)+βHCC(32)
32	A			1495	1496	2.38	4.7715	βHCH(41)+βHCC(23) +δCHCH(23)

33	A	1511		1521	1521	2.42	4.2765	β HCC(33)+ β CCC(22)
34	A			1617	1617	2.58	16.1349	vCC(39)+ β CCC(11)
35	A	1649	1664	1648	1648	2.63	60.4469	vCC(66)
36	A	2222	2334	2230	2230	3.71	390.9454	vNC(89)+ vCC(11)
37	A	3064		3033	3033	4.83	195.3965	vCH(99)
38	A	3065		3084	3083	4.91	63.8787	vCH(98)
39	A			3116	3116	4.97	55.0693	vCH(81)
40	A			3179	3179	5.07	73.9126	vCH(91)
41	A			3203	3203	5.1	162.9662	vCH(91)
42	A			3212	3212	5.12	85.3282	vCH(99)

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

vibrations. The scenery of the substituent does not align because of these stretching vibrations. The stretching has most feasible frequency between the regions at 3100-3000 cm^{-1} ¹⁸. The calculated stretching vibrations of the title compound region, in between 3202-3005 cm^{-1} . There is no experimental frequencies have been observed. The calculated CH in-plane bending vibrations of 5F2MLBN occurs in the region of 1550-1000 cm^{-1} and observed FTIR at 1511, 1459, 1142, 1051 cm^{-1} ¹⁹. The CH out-of-plane bending occurs at the region 1100-800 cm^{-1} generally. The calculated out-of-plane bending vibrations of 5F2MLBN are found at 819, 887, 1081 cm^{-1} . Observed FTIR and FTR spectra occurred 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.

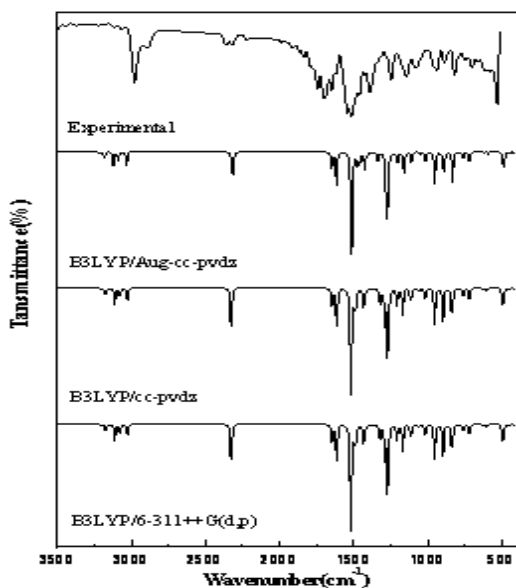


Fig. 2. Experimental and theoretical DFT/B3LYP FT-IR of 5F2MLBN

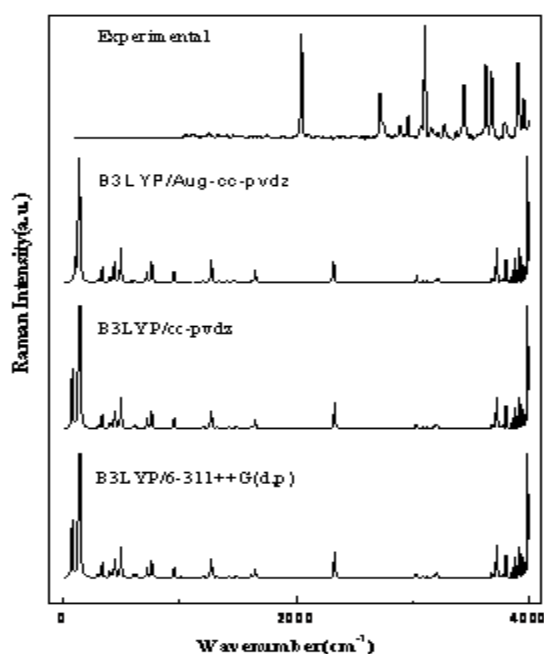


Fig. 3. Experimental and theoretical DFT/B3LYP FTR of 5F2MLBN

CF vibrations

CF moieties have been tabulated on the basis of calculated energy distribution and separated three kinds of modes. Three stretching and two in-plane bending vibrations are packed in the CF atom. The CF stretching and bending vibrations are incorporate with each other. In the literature survey, the authors assigned vibrations frequency range of 1275–412 cm^{-1} while the Carbon interactions with others heavy atoms like Cl, F, I. The 5F2MLBN compound has the strong both vibrations in the region of 1247, 937 and 1278, 944 cm^{-1} found from IR and Raman spectrum, respectively. Torsion vibrations calculated

frequency of the title molecule transpire in the range at 965, 838, 627, 337, 154 cm^{-1} . These vibrations are very well agreed with literature survey²⁰.

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 substituent²¹. 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} ²² and it is being attributes to Ca=N stretching. FL 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. These electron acceptor groups are the main impact for the shifting for Ca=N vibrational wave number. FTIR and FTR spectra frequency at 2222 and 2334 cm^{-1} for C=N (ν) vibrations found for 5F2MLBN, respectively. The calculated wavenumbers of stretching vibrations at 2230 cm^{-1} coincide with the FTR value. This is the ideal frequency of the whole molecule which confirmed the CN stretching with 89% assignment. The bending vibrations (β) of the molecule for FTIR spectra spotted at 578 cm^{-1} . 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. 9, 11, 15, 16, 19, 21, 23, 24, 26, 28, 30, 34, 35, 36) carbon vibrations slouch in the region 400-2300 cm^{-1} and thirteen bending of vibrations slouch above the region 1300 cm^{-1} ²³. 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 2222, 1649, 1459, 1390, 1247, 1142, 937, 750, 531 cm^{-1} and the five FTR at 2334, 1664, 1278, 944, 758, 434 cm^{-1} coincides each other. The

recorded spectral values of C-C-C bending modes at 1511, 937, 750, 531 and 944, 758, 434, 144 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 reports²⁴. The IR and Raman spectra peak observe in the region at 701, 666 cm^{-1} and 708, 484 cm^{-1} , respectively. These peaks have been calculated at the region at 720, 627, 492, 403, 154, 130 cm^{-1} by B3LYP methods which are well merge with observed values. And these wavenumbers are mixed with CCCN torsions in the investigated molecules.

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 5F2MLBN 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 circuits²⁵. The first hyperpolarizability (β) polarizability (α) and anisotropy of polarizability²⁶ ($\Delta\alpha$) of 5F2MLBN is calculated using DFT with the above basic set and can be evaluated using equations (1) (2) (3) respectively. The Table. 4 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 mechanisms²⁷.

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

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

$$\Delta\alpha = \frac{1}{\sqrt{2}} [(\alpha_{xx} - \alpha_{yy})^2 + (\alpha_{yy} - \alpha_{zz})^2 + (\alpha_{zz} - \alpha_{xx})^2 + 6\alpha_{xz}^2 + 6\alpha_{xy}^2 + 6\alpha_{yz}^2]^{\frac{1}{2}} \quad (3)$$

$$\beta = [(\beta_{xxx} + \beta_{yyy} + \beta_{zzz})^2 + (\beta_{yyy} + \beta_{zzz} + \beta_{xxx})^2 + (\beta_{zzz} + \beta_{xxx} + \beta_{yyy})^2]^{\frac{1}{2}} \quad (4)$$

Table. 4 : Optical properties of 5F2MLBN

Parameters	B3LYP	Parameters	B3LYP
μ_x	0.8197256	β_{xxx}	80.156319
μ_y	-0.01	β_{xxy}	-2.4476356
μ_z	1.3473167	β_{xyy}	26.3796534
μ	1.577Debye	β_{yyy}	-8.36091
α_{xx}	101.757788	β_{xxz}	-35.3219987
α_{xy}	-0.3604599	β_{xyz}	6.6626508
α_{yy}	53.7128032	β_{yyz}	28.5648953
α_{xz}	-4.5871788	β_{xzz}	21.4224614
α_{yz}	0.28	β_{yzz}	3.8015823
α_{zz}	128.7684006	β_{zzz}	-81.8304551
α_0	198.393x10 ⁻³³ esu	β_0	1345.907x10 ⁻³³ esu
\dot{A}	1713.98x10 ⁻³³ esu		

The calculated values of α and β are 1713.98x10⁻³³esu and 1345.907x10⁻³³esu. Ideal molecule urea is used for determined the comparative purpose. The compound has the values 1.577D and 1345.907x10⁻³³esu of μ and β respectively. The μ of compound is approximately 1.15 times greater than that of urea and the μ of compound is 3.62 times greater than that of urea (μ and β of urea are 1.3732 Debye and 0.3728 x10⁻³⁰esu 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 research²⁸.

CONCLUSION

From the DFT methods by three 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 α values of the compound were 1.15 and 3.62 times greater than that of urea, respectively. These properties show that the title compound 5F2MLBN had good chemical stability, bioactivity and optics applications are helping the future researchers and innovative thinkers.

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