Vibrational Frequencies, NBO Analysis, NLO Properties, UV-Visible and Homo-Lumo Analysis of 2-Chloro-3-Methoxybenzonitrile with Experimental (FT-IR and FT-Raman) Techniques and Quantum Mechanical Calculations

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ABSTRACT

Structural, Vibrational, Electrical, optical and Stability studies of 2-Chloro-3-Methoxybenzonitrile (2C3MOBN) has pore over by computational methods. The equilibrium geometry (atomic length, atomic angle and dihedral angle), frequency vibrational assignments, IR activities and Raman intensities in scattering bustles was premeditated by B3LYP method employing 6-311 ++G (d, p) / (2d, p) as the basis sets. The Raman and IR spectra of FMBN are traced and the frontier orbital energy gap has predicted. The electrostatic potential, contour map and electron density have also drawn to clarify the electronic activity of 2C3MOBN. For the future applications in non-linear optics (NLO) of the molecule has investigated threw the hyper polarizability (β) and electric dipole moment (μ) of 2C3MOBN are calculated using second basis set on the finite-field approach denote above. Intra Charge Transfer (ICT), hyper conjugative interactions, charges delocalization of the molecule has explored by Natural Bond Orbital (NBO) Fock matrix cram on the way to locate the Stability. Mulliken population analysis and Natural population analysis on charges also evaluated. Eventually investigate thermodynamic parameters like enthalpy, Gibbs free energy, zero point energy, entropy, heat capacity, dipole moment, and atomic charges.

KEY WORDS: 2-Chloro-3-Methoxybenzonitrile, Natural Bond Analysis (NBO), Atomic charges, Intra Charge Transfer and Molecular Electrostatic Potential contours/surfaces.

1. INTRODUCTION

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 Lewis (2007), and boiling point at 190.7^{0}C at 760 mm Hg (O'Neil, 2013). Benzonitrile compounds are the origin of many compounds like benzoguanamine, pesticides, intermediates of aliphatic amine and benzoic acid (Petra Lovecka, 2015). In alkali condition, Benzonitrile fabricate the benzoguanamine which is the superiority of melamine plastic is to a great extent better through and benzoguanamine resin used for coating, adhesives, laminate board and moulding materials. Organic benzonitrile act as solvents and non-aqueous solvents for greasy sours, lubricates, fragrances, unsaturated hydrocarbons, pharmaceuticals, spinning, casting and titrations of inorganic salts. Benzonitrile act as a removing agent, High pressure liquid, chromatographic analysis, recrystallization agent of steroids and which is the constituent of change-metal complex catalysts, preservative for chlorinated solvents. Methylbenzonitrile is worn in a variety of fields akin to pharmaceuticals, dyes, brightening agents, rubber chemicals. 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.

Benzoic acid reacts with lead thiocyanates, Benzonitrile phenyl cyanic compound will produced by heating (Virendrakumar, 2010). 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 century. Benzoic acids used for the production of Whitefield's ointment, tincture and Friar's balsam (Charles, 2004). The vitamin B complex had benzoic element derivatives which be present extensively in plants and animal tissues as well as utilized in contrast urology media, assess the cholocystrographic, miticides and in the pharmaceuticals assembles (Ramalingam, 2008; Balachandrana, 2004).

Several BN applications of there, e.g. 3-ethyl BN and Vamicamide (a new antichloinergic agent synthesis from BN) for the treatment of urge urinary incontinence (UUI) (Buteru, 2000; Sundaraganasan, 2009), The cardiovascular scheme of rats, used p-hydroxy for the reason that which has alpha blocker possessions (Cheav, 1998), 3-chloro BN and 4-chloro BN are the high-quality corrosion control agents of the steel, because it has the inhibition of the hydrogen absorption in addition to since enhance the absorption of hydrogen use the 2-chlrobenzonitrile.

Density Functional Theoretical modeling of methyl benzonitrile have reported by Virendrakumar (2010), contain testimony the molecular structure and vibrational spectra of 2-Chloro-6-methylbenzonitrile. Both observed and calculated methods on structural and vibrational spectra of 2-fluoro-6-methoxybenzonitrile (FMBN) have

accounted by Murugan (2012). The many derivatives using ab-initio HF / DFT methods B3LYP level deliberated the equilibrium functions, electronic plots and hyper polarizability of organic dye sensitizer 4-methoxybenzonitrile was reported by Prakasam (2013). Molecular energy stability calculations, vibrational analysis, electronic transitions and energy eigenvalues are evaluated for 2-Bromo-4-Methylnezonitrile compound done by Muhammad Shahid (2009). Literature demonstrating indicated with the function of computational studies on the 2C3MOBN element has not up till now been reported. Consequently meticulous investigations of structural properties and vibrational spectral psychiatry of the 2-Chloro-3-Methoxybenzonitrile (2C3MOBN) molecule are accepted out in the current cram by means of density functional theory (DFT) computations.

Computational details: The GAUSSIAN 09W program is used for predicted the quantum computational calculations of 2C3MOBN (Govidasamy, 2014), with the original version with three parameter functional by way of applying ab-initio Becke-Lee-Yang-Parr hybrid method in correlations B3LYP level with different basis sets on Intel Core i3 1.9GHz processor personal computer to derive the complete geometry optimization (Frisch, 2009). 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 (Saravanan, 2015). 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. Optimized geometry is given in Fig.1. 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 program. The vibrational modes are assignments are calculated and explained using the Scaled quantum mechanical program using VEDA.4.0. Software. 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.

The electronic oscillatory frequency and electronic properties such as HOMO (higher occupied molecular orbital) and LUMO (lowest unoccupied molecular orbital) orbital energy distribution, Mulliken atomic charge distribution, Natural population analysis and thermo dynamical parameters are resolute by the time-dependent DFT (TD-DFT). The energy absorption spectra and energy gap plot drawn from Gauss view 5.0 programs. Electrostatic Potential map had been drawn by MOLKEL. Bond interactions and electron high density delocalization are analyzed using NBO in Gaussian09 DFT with same basic sets. The polarizability and hyper polarizibility is calculated to understand the frequency doubling the SHG behavior of 2C3MOBN. At last investigate the density of states of different atoms, total density of states and band gap studies are investigated using theoretical replicas.

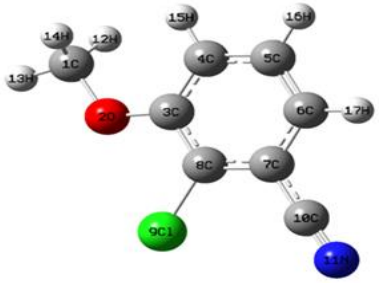

Figure.1. Optimized structure of 2C4MOBN

2. EXPERIMENTAL DETAILS

The compound 2C3MOBN was provided a sturdy purity of larger than 99% and used as such as without any additional refinement by Sigma-Aldrich Chemical Company, the USA. The FT-Raman spectrum of 2C3MOBN has been recorded using 1064nm line of Nd: YAG laser as excitation wavelength in the region 50-3500 cm^{-1} on a EZRaman, Enwaveoptronics, USA IFS 66 V spectrometer. The Fourier transform infrared (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.1 & Fig.2, shows the association of both observed and calculated IR and Raman spectra of 2C3MOBN. 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 B3LYP with 6-311++G (d, p)/ 6-311++G (2d, p) basic sets and the output spectra are monitored threw Gauss sum program, which gives the Raman intensities spectra directly. 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.

3. RESULTS AND DISCUSSION

Molecular Geometry: The equilibrium geometrical parameters namely atomic lengths, atomic angles and dihedral angles calculated by dissimilar levels are listed in Table.1. The predicted geometrical optimized molecular structure of 2C3MOBN has 16 atoms among 42 symmetry species of vibrations that are obtained chemcraft program is shown in Fig.1. The microwave data for benzonitrile data are compared with the optimized structural parameters. The theoretical geometrical parameters are fruitful concurrence with experimental method. The atomic lengths of carbon and carbon atoms had seven interactions, these are calculated as 1.40 Å and their corresponding recorded values (Microwave Data) are 1.38 Murugan (2012), respectively. All the carbon-carbon interactions have similar bond length. The carbon-hydrogen has six interactions and these bond lengths are C1-H12, C1-H13, C1-H14, C4-H15, C5-H16 and C6-H17 calculated are 1.07 Å and their corresponding recorded values (Microwave Data) are 0.93 Å respectively. Which denotes the benzene ring is appearing. In 2C3MOBN, the chloride had main element and place a vital role. For the chloride-carbon (C8=Cl9) group bond length is observed at 1.76 Å this value exactly matches with the literature (Virendrakumar, 2010), the length of bond between Carbon-Nitrogen group was observed at 1.16Å and the computed value is 1.15Å, it found support from the literature (Casado, 1971). The hexagonal structure of the bond angles between all atoms that has almost the same and microwave data also merged.

The bond angle of C7-C8-Cl9 and C3-C8-Cl9 are calculated and observed values are about 120.2° and 120.1° respectively. The bond angle of C7-C8-Cl9 has largest value about 120.2° and O2-C1-H12 has smaller value about 109.2°. The calculated geometric optimized parameters can be applicable for determine the other parameters like Natural Band Orbital (NBO) and NLO of 2C3MOBN.

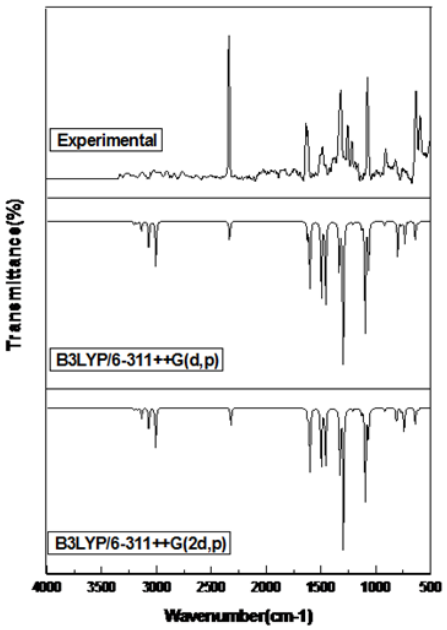

Figure.2. Experimental & calculated FTIR spectrum

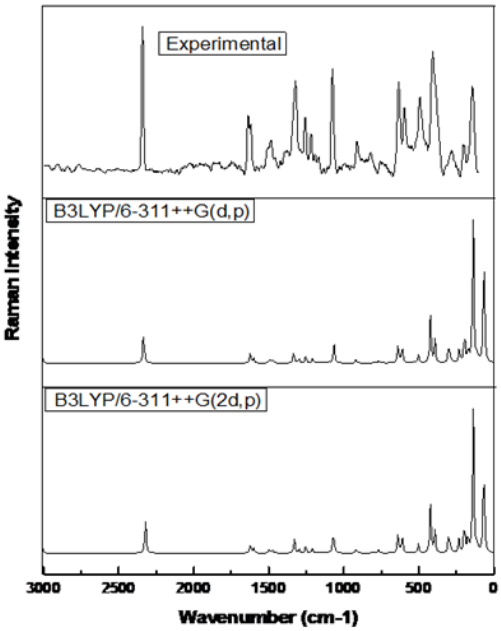

Figure.3. Experimental & calculated FT-Raman spectrum

Vibrational Assignments: 2-Chloro-3-Methoxybenzonitrile molecules contain 16 atoms and possessions to the point group Cs. The three Cartesian displacements of the 16 atoms offer 48 internal modes. The entire the elementary vibrations are vigorous in cooperation IR and Raman. Every vibrations intended for N atomic molecules had 2N-3 and N-3 is in-plane and out of plane respectively. As a result 13 in-planes and 11 out of plane bending are identified for 2C3MOBN 29 of all 42 vibrations.

In the novel compound of 2C3MOBN are premeditated the harmonic vibrational frequencies at B3LYP level by various basis sets have specified in Table.2. From that table has obtained the pragmatic IR and Raman frequencies for an assortment of modes of vibrations are Contrast of the frequencies designed by B3LYP functional tends to misjudge the essential modes. It is observed that scaling factor has to be used for obtaining the substantial healthier conformity among 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 properties such as (reduced mass, force constants, depolarization ratios) as well as IR & Raman intensities of the title molecule. In Figs.2 & 3, shows the comparisons of experimental and calculated spectra.

C-H Vibrations: The characteristically make obvious as weak to reasonable bands which this vibrations take place higher than 3000 cm^{-1} (Suhasini, 2015). The C-H stretching modes more periodic does not am within view with lucrative Raman term and are intensively polarized. May be guerdon to this fancy polarization, Raman band has been efficient in concealed spectra and this vibrations of benzene derivatives constantly become clear as a bell above 3000cm^{-1}. From this vibration has found the vibrations of appetizing ring from the IR spectrum of 2C3MOBN the

shoulder strap of 3015 and 3076cm^{-1}. For the Raman spectra observed almost same the band at 3014 and 3076cm^{-1} are attributed to the vibrations. The computed vibrations in the 3212-3014cm^{-1} are in agreement with experimental assignment 3213-3015cm^{-1} (Frisch, 2009). The three in plane C-H bending vibrations appear in the range 1000-1300cm^{-1} for the substituted benzenes and the three out of plane bending vibrations occur in the frequency range 750-1000cm^{-1}. In general, the weaker intensity is malformed in higher Wavenumbers of the C-H plane out-of-plane than lower one. This research articles leads to the out-of-plane vibrations are identified in this stretching for the both spectrum and which are expected to interact a little around 1600 – 1300 cm^{-1} with ring vibrations.

Hypothetically computed vibrational frequency calculated by the high technique 1071, 1097, 1132, 1170, 1197, 1212, 1256, 1300 cm^{-1} (modes 30-23) are assigned to the in plane bending vibrations. In the intensity value as the measured frequencies 973, 919, 891, 814, 768 and 743cm^{-1} (modes 22-17) by the same basis set for this out of plane bending vibrations.

C=O vibrations: The observed region 1700–1660 cm^{-1} is the best frequency vibration for carbonyl group. For the reason that of its sky-scraping intensity and the comparatively interference-free province in which it occurs, this band is logically effortless to distinguish. Asha Raj (2009), assigned vibrations of C-O band observed at 1330 cm^{-1} (DFT) and 1336 cm^{-1} (Raman) as the stretching mode. Suhasini (2015), 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 1624, 1604 cm^{-1} in the IR spectrum and 1627 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 (Casado, 1971). The 2-(MCMS)-3, 5-DNB Carboxylic Acid has observed at1336 cm^{-1} in (C-O) stretching mode. For the title compound, has assigned the stretching at 1332 cm^{-1}(DFT) and 1336 cm^{-1} (Raman).

C≡N vibrations: The 1627–1566 cm^{-1} range are observed in the C≡N stretching skeletal bands. From the nitrogen compounds had triple or doubled bounds like cyanides with a single spectrum classically absorption at 2280-2200cm^{-1} and 2285-1990cm^{-1} for cyanates, isocyantes and thiocyanates with a single normally intense. In the phenyl ring, the cyano group is the novel substituent while exaggerated considerably. The benzonitrile molecule does not affected by the vibrational wave numbers on the cyano group. Electron withdrawing groups such as –Cl, -O, -Br, -CN and -OH decrease the IR band intensity and increase the wave numbers value to the higher limit of the characteristics spectral regions, whereas electron donating groups, such as amino group, increase the intensity and decrease the wave numbers. The C≡N stretching vibrations is attached to the aromatic ring had good intensity has observed at 2240-2221cm^{-1}. Our title compound 2C3MOBN has the IR band at 2236cm^{-1} indicates this stretching vibration. The computed and assigned by the Gauss view package at 2236cm^{-1} by a variety of basis set (mode no.39) is assigned to this stretching vibrations. This group has in-plane and out-of-bending modes which gives the contrast appear with the IR intensity and with null Raman activity and strongly coupled with C-C-C bending modes. Contribution of the in-plane bending mode are resolute in the bands at roughly 600, 550 and 30 cm^{-1} while the out-of-plane mode is identified in the IR band at 423 cm^{-1}, in contradiction with that reported in MFBN (Murugan, 2012) at 606 cm^{-1}. Hence in the present study, the C≡N in-plane and out-of- plane bending modes are recorded at 629 cm^{-1} in FT–IR. These bands are in good agreement with the calculated values are found at 628 cm^{-1}.

C–C vibrations: Benzene ring had six equivalents and consequently C-C bonds and CC-Stretching vibrations also exist. In addition, the carbon ring had several kinds of vibrations at the in and out-of-plane bending. Both observed IR and Raman spectra covering the spectral range from 1600 to 1400 cm^{-1} in the C–C aromatic stretching vibrations give rise to characteristic bands. The calculated values of C–C stretching vibrations are found to be 1604, 1503, 1501, 1496, 1476 and 1461 cm^{-1} in first basic set, 1604, 1502, 1498, 1495 and 1459 cm^{-1} in second basis set already said above. These calculated bands are in first-class correlation with the experimental observations of values.

C–Cl vibrations: The main reason of that the subordinating the molecular symmetry and heavy particles subsist in the molecules, these on the margin has amalgamation of vibrations are possible which is because of exist in the molecules has bonding of the ring and halogen (chlorine) atoms. And which benzene complex are prepared by the potential energy distributions of C-Cl group vibrations. Mooney (1963 & 1964), observed wave number range of 1129–480 cm^{-1} of Bromide, Carbon-chloride and Iodine. These stretching vibrations give generally strong bands in the region 710–505 cm^{-1}. For simple organic chlorine compounds, C–Cl absorptions are in the region 750–700 cm^{-1}. Virendrakumar (2010), observed at 871 cm^{-1} of C–Cl vibrations at Raman spectrum calculated the value at 842cm^{-1} has identified the stretching corresponding too theoretically. Prasad (2015), assigned vibrations of C–Cl band observed at 1045 cm^{-1}. Sawant (2013), assigned vibrations of C–Cl band observed at 740 cm^{-1}.The out-of-plane deformation vibration has established at 190 cm^{-1} by both vibrational spectrum. For the title compound, the stretching mode was assigned the band observed at 890 cm^{-1} (mode No.20) for both spectrums in addition to 891 and 893 cm^{-1} in the theoretically for two basis sets respectively. The deformation bands are also identified and these results associate with the literature data (Virendrakumar, 2010). For 2-CPCDC compound observed at 870 cm^{-1}, 877 cm^{-1} (IR, Raman) and 882 cm^{-1} is reported theoretically.

Table.1. Optimized geometrical parameters of 2C3MOBN

Parameters	B3LYP/6-311++G		Microwave Data(benzonitrile)	Parameters	B3LYP/6-311++G	
Bond Length (Å)	(2d ,p)	(d, p)		Dihedral Angle (°)	(2d, p)	(d, p)
C1-O2	1.43	1.43		H12-O1-C2-C3	60	60
C1-H12	1.07	1.07	0.93	H13-O1-C2-C3	180	180
C1-H13	1.07	1.07	0.93	H14-O1-C2-C3	-60	-60
C1-H14	1.07	1.07	0.93	C1-O2-C3-C4	-30	-30
O2-C3	1.43	1.43		C1-O2-C3-C8	150	150
C2-C4	1.40	1.40	1.379	O2-C3-C4-C5	180	180
C3-C8	1.40	1.40	1.379	O2-C3-C4-H15	0	0
C4-C5	1.40	1.40	1.379	C8-C3-C4-C5	0	0
C4-H15	1.07	1.07	0.93	C8-C3-C4-H15	180	-180
C5-C6	1.36	1.40	1.375	O2-C3-C8-C7	180	180
C5-H16	1.07	1.07	0.93	O2-C3-C8-C9	0	0
C6-C7	1.40	1.40	1.379	C4-C3-C8-C7	0	0
C6-H17	1.07	1.07	0.93	C4-C3-C8-C9	180	180
C7-C8	1.40	1.40	1.379	C3-C4-C5-C6	0	0
C7-C10	1.40	1.40	1.379	C3-C4-C5-H16	-180	180
C8-Cl9	1.76	1.76	1.74	H15-C4-C5-C6	180	180
C10-N11	1.15	1.15	1.156	H15-C4-C5-H16	0	0
Bond Angle(°)				C4-C5-C6-C7	0	0
O2-C1-H12	109.5	109.5	109.2	C4-C5-C6-H17	180	-180
O2-C1-H13	109.5	109.5		H16-C5-C6-C7	180	-180
O2-C1-H14	109.5	109.5		H16-C5-C6-H17	0	0
H12-C1-H13	109.5	109.5		C5-C6-C7-C8	0	0
H12-C1-H14	109.5	109.5		C5-C6-C7-C10	-180	180
H13-C1-H14	109.5	109.5		H17-C6-C7-C8	180	180
C1-O2-C3	109.5	109.5		H17-C6-C7-C10	0	0
O2-C3-C4	120.2	120.0		C6-C7-C8-C3	0	0
O2-C3-C8	120.2	120.0		C6-C7-C8-Cl9	180	180
C4-C3-C8	119.6	120.0		C10-C7-C8-C3	-180	180
C3-C4-C5	120.0	120.0	120.2	C10-C7-C8-Cl9	0	0
C3-C4-H15	120.0	120.0				
C5-C4-H15	120.0	120.0				
C4-C5-C6	120.4	120.0	119.5			
C4-C5-H16	119.8	120.0				
C6-C5-H16	119.8	120.0				
C5-C6-C7	120.4	120.0				
C5-C6-H17	119.8	120.0				
C7-C6-H17	119.8	120.0				
C6-C7-C8	120.0	120.0				
C6-C7-C10	120.0	120.0				
C8-C7-C10	120.0	120.0				
C3-C8-C7	119.6	120.0				
C3-C8-Cl9	120.2	120.0	120.1			
C7-C8-Cl9	120.2	120.0	120.1			

Microwave Data (benzonitrile)

Table.2. vibrational frequencies of 2C3MOBN

Symentry Spices	Calculated frequency B3LYP/6-311++G (cm-1)		Observed frequency (cm^{-1})				
	(2d, p)	(d, p)	IR	Raman	IR Activity	Raman Intensity	Vibrational Assignments
A	68	67			0.01	5621.24	CCCN out-of-plane bending

A	113	111		112	6.13	325.29	C-OCH_3 out-of-plane bending
A	137	138		136	2.35	8140.91	CCN rocking, CCC in-plane bending
A	173	172		172	0.37	930.28	CCl out-of-plane bending, CCN out-of-plane bending
A	197	196		196	0.92	1703.82	CCCN torsion, CCCCl torsion, CCCC torsion
A	233	230			0	761.20	ClCCC out-of-plane bending, NCCC torsion, CCCC out-of-plane bending, NCCC out-of-plane bending
A	287	285		286	0.2	295.93	CCCl in-plane bending, NCC in-plane bending, CCC in-plane bending
A	302	301		302	3.34	1145.18	ClCC in-plane bending, NCC in-plane bending,CCC in-plane bending
A	394	394		394	0.27	1300.83	Ring in-plane, CCN torsion
A	423	424		422	3.07	2681.03	trigonal deformation, torsion ring asymm
A	427	426		426	3.76	201.37	Ring (CN) symm in-plane bending
A	505	504	505		1.08	464.33	CN in-plane bending
A	538	533	537	536	0.18	36.25	CN torsion, CCCC out-of-plane bending, ClCCC out-of-plane bending
A	612	612	612	612	2.4	979.96	CCC out-of-plane bending
A	629	630	628	628	1.4	147.14	CCCC out-of-plane bending, CCl stretching (1)
A	641	640	640	640	19.26	994.09	CCCC out-of-plane bending, CCl stretching (2)
A	743	736	742	742	35.47	1.94	CCC in-plane bending
A	768	767	768	768	5.12	179.18	C-CN ring symm stretching
A	814	802	814	814	23.38	45.02	C-H out-of-plane bending
A	891	893	890	890	0.01	7.36	C-H out-of-plane bending
A	919	920	918	918	4.39	235.03	CH symm out-of-plane bending
A	973	976	972	972	0.36	0.57	Trigonal breathing, O–CH3 bending
A	1071	1068	1070	1070	49.59	1275.17	CH (ortho) in-plane bending, ring in-plane deformation
A	1097	1098	1096	1096	114.03	32.28	CC asymm stretching (2)
A	1132	1132	1132	1132	7.59	25.04	CH_3 rocking yz plane
A	1170	1168	1170	1170	0.95	49.64	CH (ortho) in-plane bending, ring in-plane deformation
A	1197	1195	1196	1196	0.55	19.67	CH (para) in-plane bending out-of-plane
A	1212	1210	1212	1212	2.84	270.73	CH in-plane bending, CC in-plane bending
A	1256	1256	1256	1256	0.75	466.14	CH in-plane bending C–O stretching
A	1300	1301	1300	1300	170.42	193.97	CH in-plane bending, CC stretching
A	1332	1336	1332	1332	76.28	767.65	CH in-plane bending CC stretching

A	1461	1459	1460	1460	74.66	13.16	CH_3 bending asymm, CC stretching, CH in-plane bending
A	1476	1474	1476	1476	2.19	141.17	CH_3 bending asymm
A	1496	1495	1496	1496	9.72	163.78	CH_3 out-of-phase deformation
A	1501	1498	1500	1500	38.9	27.90	CC symm stretching,CH in-plane bending
A	1503	1502	1502	1502	38.55	52.62	CC symm stretching,CH in-plane bending
A	1604	1604	1604	1604	73.23	269.97	CC symm stretching, CO stretching
A	1624	1627	1624	1624	13.83	548.48	CC stretching, CCC in-plane bending
A	2326	2338	2326	2326	22.34	1942.69	CN ring symm stretching
A	3015	3013	3014	3014	46.25	356.21	CH symm stretching xz plane
A	3076	3076	3076	3076	27.19	116.90	CH ring symm stretching
A	3142	3145	3142	3142	12.37	199.58	CH ring symm stretching
A	3184	3185	3184	3184	3.56	129.87	CH ring symm stretching
A	3206	3208	3206	3206	1.17	148.45	CH ring symm stretching
A	3213	3213	3212	3212	2.67	281.18	CH ring symm stretching

Table.3. IR intensities (km mol^{-1}), Raman intensities (Å4 amu^{-1}), reduced masses (amu), force constants (m dyne Å^{-1}), depolarization ratios (polarization (P) and unpolarized (U)) are obtained for 2C3MOBN calculated by B3LYP/6-311++G (2d, p) basis set

No.	IR intensities	Raman intensities	Reduced masses	Force constants	Depolarization ratios	
					P	U
1	0.0099	5621.24	4.5605	0.0123	0.75	0.8571
2	6.128	325.29	5.317	0.0401	0.75	0.8571
3	2.3482	8140.91	11.6955	0.13	0.7183	0.8361
4	0.3731	930.28	3.458	0.0611	0.75	0.8571
5	0.9162	1703.82	6.1403	0.1399	0.6372	0.7784
6	0.0022	761.20	1.4751	0.0473	0.75	0.8571
7	0.2033	295.93	2.7505	0.1334	0.75	0.8571
8	3.3357	1145.18	4.3941	0.2354	0.4403	0.6114
9	0.2739	1300.83	11.7926	1.0799	0.5744	0.7297
10	3.0714	2681.03	6.8725	0.7256	0.1008	0.1831
11	3.7622	201.37	6.9553	0.7486	0.7498	0.857
12	1.0764	464.33	8.4747	1.2725	0.576	0.731
13	0.1764	36.25	3.9487	0.6738	0.75	0.8571
14	2.4023	979.96	7.4341	1.639	0.1882	0.3167
15	1.3972	147.14	5.5515	1.294	0.75	0.8571
16	19.2561	994.09	5.176	1.2522	0.0603	0.1138
17	35.4749	1.94	1.5999	0.52	0.7499	0.8571
18	5.1243	179.18	7.0123	2.4373	0.5274	0.6906
19	23.3807	45.02	2.9583	1.1544	0.75	0.8571
20	0.0076	7.36	1.4297	0.6692	0.7499	0.8571
21	4.3874	235.03	6.2319	3.1014	0.3005	0.4622
22	0.3592	0.57	1.3217	0.7369	0.7499	0.8571
23	49.591	1275.17	6.4704	4.3693	0.0694	0.1297
24	114.0287	32.28	7.0156	4.9734	0.088	0.1618
25	7.5946	25.04	1.8306	1.3827	0.1738	0.2961
26	0.9534	49.64	1.2706	1.025	0.75	0.8571
27	0.551	19.67	1.2985	1.0962	0.7495	0.8568
28	0.8439	270.73	1.3104	1.1332	0.5878	0.7404
29	0.7499	466.14	2.4411	2.267	0.1357	0.239
30	170.4225	193.97	3.7239	3.7062	0.1465	0.2556
31	76.2789	767.65	5.6205	5.8713	0.2116	0.3493

32	74.6597	13.16	2.534	3.1859	0.7414	0.8515
33	2.19	141.17	1.5733	2.019	0.307	0.4698
34	9.7157	163.78	1.0458	1.3798	0.75	0.8571
35	38.8973	27.90	1.9198	2.5472	0.667	0.8002
36	38.5474	52.62	1.0854	1.4445	0.722	0.8386
37	73.231	269.97	4.8858	7.4016	0.6867	0.8142
38	13.8349	548.48	6.5195	10.1361	0.5978	0.7482
39	22.3438	1942.69	12.6843	40.4492	0.2644	0.4182
40	46.2524	356.21	1.034	5.5368	0.0293	0.0569
41	27.1856	116.90	1.1069	6.1723	0.75	0.8571
42	12.3746	199.58	1.1	6.3998	0.4672	0.6368
43	3.561	129.87	1.0881	6.5005	0.5385	0.7
44	1.1679	148.45	1.0925	6.6176	0.4376	0.6088
45	2.6709	281.18	1.0933	6.6479	0.1243	0.2211

Methyl group vibrations: The title molecule 2C3MOBN under deliberation possesses the ring has only one CH_3 group in second position. For the assignments of CH_3 group frequencies, one can expect nine fundamentals can be associated to each, namely the symmetrical stretching (CH_3 sym. stretch) and asymmetrical stretching (CH_3 asym. stretch), in-plane stretching modes (i.e, in-plane hydrogen stretching mode); the symmetrical (CH_3 sym. deform) and asymmetrical (CH_3 asy. deform) deformation modes; the in-plane rocking (CH_3 ipr), out-of-plane rocking (CH_3 opr) and twisting (tCH_3) modes. Methyl groups are generally referred as electron donating substitution in the aromatic ring system.

At about 1475-1432 cm^{-1} both the deformations of these groups are calculated, as listed in the Table.3, and in the 1070-1010 cm^{-1} range the methyl group rocking modes Guru Prasad (2013). The rocking modes are calculated below 1192 cm^{-1}. It is seen that the transport of the scale factors reproduces the predictable experimental behavior of the methyl group. Some bands corresponding to the methyl group fundamentals are not experimentally observed. For example, of the bands corresponding to the das (CH_3) modes, only the bands at about 1461, 1476, 1496, 1501, 1503, 1604 and 1624 cm^{-1} are observed in 2C3MOBN. The rocking vibrations of (CH_3) have been identified at 1070cm^{-1} i.e. the theoretically calculated value by hybrid method using the two basis set is at 1071 and 1068 cm^{-1} respectively. The both deformations in-plane bending modes of this group are at 1332 and 1300 cm^{-1} (mode no.31 and 30). Likewise, a medium strong FT-Raman band observed at 1170 cm^{-1} (mode no.26) with mixed contribution to the υCC, with no FT-IR band observed in 2C3MOBN molecule has been assigned to out-of-plane deformation.

In the research paper have found that the vibrational bands corresponding to methyl vibrations virtually stay put the equal in magnitude and intensity. Methyl rocking frequencies are mass sensitive and variable in position due to the interaction through skeletal stretching modes. Normally, these bands are observed weakly in the range 1120-1050 cm^{-1} and 900-800 cm^{-1}. For the FMBN, only a very strong FT-IR band at 1097 cm^{-1} combined with computed ones have been assigned, since the medium FT-IR band at 891 cm^{-1} with significant contribution to the β Rtrigd and Rtrigd, which have been assigned to in-plane rocking and out-of-plane rocking modes, respectively. As CH_3 twisting mode is expected below 400 cm^{-1}, the computed bands at 68 cm^{-1} and 67 cm^{-1} by the two methods without support by PEDs, are assigned to this mode, for no spectral measurements were possible in the region due to instrumental limits.

Electronic Transition and HOMO-LUMO: To comprehend electronic transitions on terms of energies and oscillator strengths, calculations have carried out in the gas phase with the best basis set. Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) interactions are held between acid-base. In general, when the orbital reacts with one another is produced another two orbital which has the filled-empty interaction for the stabilization. Those interactions are most welcomed orbital in molecules for reactivity and kinetic stability. The HOMO is the orbital that could act as fulfilled electron pair, most available for bonding, most weakly held electrons and characteristic for nucleophilic component. The LUMO is the orbital that could act as the empty and characteristic for electrophilic component. These orbital are placed in a final boundary level of electron of the molecule, so it is called the frontier orbital (FMO's). HOMO energy, LUMO energy and chemical potential analyzed by the above basic sets and the energy gaps of the different stages like $EHOMO_{1,2,3}$-$ELUMO_{1,2,3}$ and related electronic properties of 2C3MOBN has been tabulated in Table.4. The bond between atomic orbital compositions is described by the electronic transition diagram shown in Fig.4.

In General a molecule could be excited by an external source (i.e. photons) and an electron can jump from an occupied state to an unoccupied state and an excited molecule. Sometimes this molecule reacts differently than the ground state molecule. For example in Ir 3+ complexes, often used as catalyst, you can have an "unspinning" process. By Irradiation with light, an electron pair (spin +1/2 1/ 2) in the highest occupied d orbital is excited and the electron jump in the unoccupied d orbital. By doing this you create 2 singlet with +1/2 spin. This now can relax also

by transferring (or taking) one of these electrons to a Legend (or the molecule attached to the catalytic Center). The process is not completely well understood, as these active Transition states, are very hot, so they have a short life, but with DFT could be simulated quite well. As what happen will depend on the detailed electronic representation and on the allowed or not allowed transitions. It suggests looking at some photochemistry literature, as there the transitions are often well described.

In our title compound has high delocalization of π -electrons which absorbed 274nm and these band is due to the electronic transition of π- π*.The benzonitrile dyes have the electron injection, especially when electrons are being injected for semiconductor. The stability for structures is the important role of the molecules which is confirmed by the energy gap between the two orbitals. The title compound had molecular charge transfer because of small energy gap is 5.11 eV and equal wavelength is 274 nm which is used as a potential source for UV light (Vinod Kumar, 2013). Energy gap is little and it is trouble-free to observe that they can be sensitive to the influence of the polar environment. The frontier orbital gap of the title compound has a small value. So this has a very high polarizability, high chemical reactivity and low kinetic stability. And generally lower orbital gap compound are the soft nature compounds. In the present study, the predicted the 2.54 Debye is the dipole moment of the compound (Table.6) which is a sign of the stronger intermolecular interactions occurs. UV–Vis spectra analyses of 2C3MOBN have scrutinized by hybrid method additionally predicted the vertical excitation energies at 4.52794 eV (273.82 nm), oscillator strength and wavelength (Table.4 & Table.5). The maximum absorption wavelength of the compound has the function of electron. The theoretically plots are presented in Fig.5. The 3D images of the orbital computed for the 2C3MOBN molecules are illustrated in Fig.4. The frontier molecular orbital's (FMO) energy parameters as well as equivalent density of state (DOS) of 2C3MOBN are shown in Fig.6.

HOMO energy (B3LYP) = 7.24eV LUMO energy (B3LYP) = 2.13eV

HOMO–LUMO energy gap (B3LYP) = 5.11eV

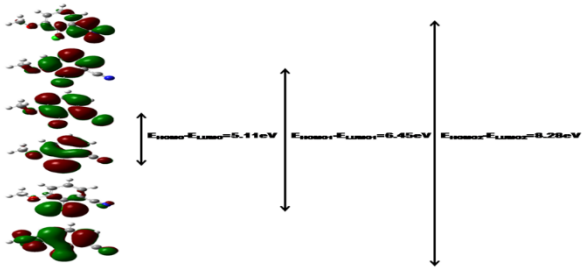

Figure.4. Molecular orbital diagram of 2C4MOBN

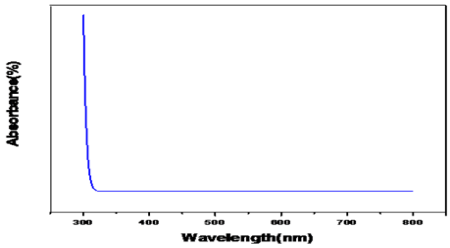

Figure.5. Calculated UV-vis Spectrum of 2C4MOBN

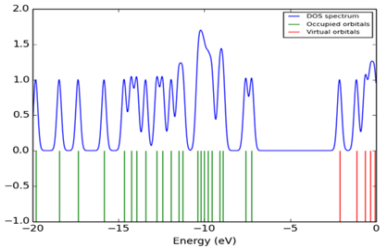

Figure.6. DOS spectrum of 2C4MOBN

The title compound 2C3MOBN has -898.748 a.u of self-consistent field (SCF) energy. At last, the lower energy gap between the molecules is the main reason for the ultimate charge transfer interactions captivating position within the molecule.

Table.4. Comparison of HOMO and LUMO energy gaps and related molecular properties of 2C3MOBN.

Molecular properties	Energy(eV)	Energy gap	Ionisation potential (I)	Electron affinity (A)
HOMO	-7.24	-5.11	-7.24	-2.13
LUMO	-2.13			
HOMO-1	-7.59	-6.45	-7.59	-1.14
LUMO+1	-1.14			
HOMO-2	-8.91	-8.28	-8.91	-0.63
LUMO+2	-0.63			
HOMO-3	-9.11	-8.78	-9.11	-0.33
LUMO+3	-0.33			
HOMO-4	-9.56	-9.48	-9.56	-0.08
LUMO+4	-0.08			
HOMO-5	-9.79	-10.05	-9.79	0.26
LUMO+5	0.26			

Global hardness (η)	Electro negativity(χ)	Global softness (σ)	Chemical potential (μ)	Global electrophilicity(ω)
2.56	-4.69	0.39	4.69	5.99
3.225	-4.365	0.310	4.365	7.038
4.14	-4.77	0.241	4.77	9.873
4.39	-4.72	0.227	4.72	10.360
4.74	-4.82	0.210	4.82	11.423
5.025	-4.765	0.199	4.765	11.972

Table.5. Energy Excitations, Wavelength and Oscillator Strength of the 2C3MOBN

S.No	Energy (cm-1)	Wavelength (nm)	Osc. strength	Symmetry
1	36520.23024	273.8208367	0.0547	A-Signlet
2	43201.77328	231.47198	0.0908	A-Signlet
3	46390.10496	215.5632113	0.0019	A-Signlet

NLO Properties: 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. The first hyper polarizability (β) polarizability (α) and anisotropy of polarizability (Δα) of 2C3MOBN is calculated using DFT with the above basic set and can be evaluated using equations (1) (2) (3) respectively. The Table 6 listed the numerical values of above mentioned parameters. In the presence of an external electric field (E), the excitation energy of the system is a function of the electric field. 3×3×3 matrix is used for determined the hyper polarizability.

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

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

$$\beta = \left[\left(\beta_{xxx} + \beta_{xyy} + \beta_{xzz}\right)^2 + \left(\beta_{yyy} + \beta_{zzy} + \beta_{yxx}\right)^2 + \left(\beta_{zzz} + \beta_{zxx} + \beta_{zyy}\right)^2\right]^{1/2} \quad (3)$$

In this research paper, 2C3MOBN compound has been computed and tabulated the polarizability. The hyper polarizability tensors are predicted only on the software with basic set and results obtained from the equations already programmed by software. The efficiency of electronic communication between acceptor and the donor groups is the best way to get the intra molecular charge transfer this is causes for the consequence of the polarizability and hyper polarizability of molecular systems (Mathammal, 2015). If the diagonal components have numerical value and nil value, which is controls the calculated polarizability (aij). The value α and β is equated as $2246.5599 \times 10^{-33}$ esu and $3242.63108 \times 10^{-33}$ esu for title molecules with best basic set respectively.

The calculated values of α and β comes out to be as 262.142a.u and 378.37a.u. Threshold values for NLO effects is that of Urea used for comparison purposes whose polarizability and first hyper polarizability values are compared with our title compound values. It has been shown the enhancing NLO property. Since from the computed results, the values are 10 times that of standard values. The recent molecule has steady state potential for NLO applications like frequency doubling and SHG that is confirmed by the recent research.

Table.6. First order hyperpolarizability of the 2C3MOBN

Parameters	B3LYP/6-311++G(2d,p)	Parameters	B3LYP/6-311++G(2d,p)
μx	0.107604	βxxx	240.4706816
μy	-0.9559419	βxxy	-34.9754167
μz	-2.36	βxyy	51.3191431
μ=	2.5485Debye	βyyy	-70.5965348
αxx	128.7858239	βxxz	1.2773559
αxy	-7.612741	βxyz	4.9642787
αyy	84.9959011	βyyz	-35.7895026
αxz	14.1543083	βxzz	68.3065216
αyz	32.6827985	βyzz	28.616343
αzz	138.773559	βzzz	-38.1842572
α0	$260.03957 \times 10^{-33}$esu	β0	$3242.63108 \times 10^{-33}$esu
α=	$2246.5599 \times 10^{-33}$esu		

NBO analysis: The high electron density in orbital bonding is predicted Natural Bond Orbital (NBO) analysis and mainly focused the stability of the molecules which makes a decision for what are the qualities exist in the molecules like The hyper conjugative interactions, inter-, intramolecular hydrogen bonding, Intermolecular Charge Transfer (ICT), electron density transfer (EDT) and cooperative effect due to the delocalization of electron density from the filled lone pairs of Lewis base 'n(y)' into the unfilled antibonding of Lewis acid 'σ*(x-H) or π*(x-H)'. In the natural localized orbital sets, NBOs is the one of the sequence. Natural localized orbital calculate the electron density in

atom and bonding of the atoms. Using the matrix evaluated the interactions of the orbital in this analysis and investigated the molecular interaction in a convenient basis set. The theory is also reported for resulting the cooperating stabilization energy and the electron donor-acceptor orbital. The just right structure into an empty non-Lewis orbital predicting the solution of interaction is a loss of occupancy from the concentration of electron bond. For each the stabilization energy E (2) allied with the delocalization i-j is estimated as:

$$E(2) = -n_\sigma \frac{\langle\sigma|F|\sigma\rangle^2}{\varepsilon_\sigma^* - \varepsilon_\sigma} = -n_\sigma \frac{F_{ij}^2}{\Delta E} \quad (4)$$

Where $\langle\sigma|F|\sigma\rangle^2$ or F_{ij}^2 is the Fock matrix element i and j orbitals, ε_σ^* and ε_σ are the energies of σ*and σ and n_σ is the population of the donor σ orbital.

Table.7. Second order perturbation theory analysis of Fock matrix in NBO basis for 2C3MOBN

Donor (i)	Type	Ed/e	Acceptor (j)	Type	Ed/e	E(2)	E(i)- E(j)	f(i,j)
C1 - O2	σ	1.99007	C3 - C8	σ*	0.0344	2.41	1.34	0.051
C1 - H12	σ	1.99359	C4 - C5	σ*	0.01625	0.55	1.09	0.022
C1 - H13	σ	1.99092	O2 - C3	σ*	0.03075	2.76	0.8	0.042
O2 - C3	σ	1.98765	C3 - C8	σ*	0.0344	0.52	1.35	0.024
O2 - C 3	σ	1.98765	C7 - C8	σ*	0.03678	1.64	1.35	0.042
C3 - C4	σ	1.97318	C3 - C8	σ*	0.0344	4.58	1.26	0.068
C3 - C4	σ	1.97318	C8 -Cl9	σ*	0.02688	4.7	0.86	0.057
C3 - C4	π	1.65246	C7 - C8	π*	0.45212	19.73	0.27	0.067
C3 - C8	σ	1.97766	C3 - C4	σ*	0.02611	3.87	1.28	0.063
C4 - C5	σ	1.97393	O2 - C3	σ*	0.03075	4.2	0.97	0.057
C4 - H15	σ	1.9746	C3 - C8	σ*	0.0344	3.95	1.08	0.058
C5 - C6	π	1.68086	C7 - C8	π*	0.45212	20.69	0.27	0.069
C5 - H16	σ	1.97758	C6 - C7	σ*	0.02685	4.41	1.06	0.061
C6 - C7	σ	1.9587	C7 - C8	σ*	0.03678	5.11	1.24	0.071
C6 - H17	σ	1.97669	C4 - C5	σ*	0.01625	4.46	1.08	0.062
C7 - C8	σ	1.9664	C6 - C7	σ*	0.02685	4.7	1.27	0.069
C7 - C8	π	1.68545	C3 - C4	π*	0.35907	19.15	0.29	0.067
C7 - C8	π	1.68545	C10 - N11	δ*	0.0746	16.8	0.4	0.078
C7 - C10	σ	1.97697	C10 - N11	σ*	0.01153	9.68	1.7	0.115
C8 -Cl9	σ	1.98574	C3 - C4	σ*	0.02611	2.53	1.24	0.05
C10 - N11	σ	1.99297	C7 - C10	σ*	0.03054	8.59	1.59	0.105
C10 - N11	δ	1.95413	C7 - C8	π*	0.45212	9.6	0.33	0.056
LP(1)O2		1.96907	C3 - C4	σ*	0.02611	4.8	1.12	0.066
LP(2)O2		1.87539	C3 - C4	π*	0.35907	18.55	0.33	0.074
LP(2)O2		1.87539	C3 - C4	σ*	0.02611	0.59	0.85	0.021
LP(1)Cl9		1.9934	C7 - C8	σ*	0.0344	1.61	1.46	0.044
LP(3)Cl9		1.91552	C7 - C8	π*	0.45212	13.87	0.31	0.065
LP(1) N11		1.9723	C7 - C10	σ*	0.03054	11.45	1.04	0.097

a E(2) means energy of hyper conjugative interaction (stabilization energy).

b Energy difference between donor and acceptor i and j NBO orbitals.

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

In the current paper, NBO analysis has been carry out on 2C3MOBN at the high level by abet of NBO9.1 program executed in the software with the purpose of explicate the intramolecular, delocalization of electron density, Table 7 has that values. The electron interactions of the molecules is the main reason for the stabilization energy E (2) and which gets increased the interaction between the electrons also had more intense. The strong stabilization energy value 20.69 kJ/mol is observed the molecule interactions for bonding π (C5-C6) and anti-bonding π*(C7–C8) and which shows the donating groups and the phenyl ring. This results in ICT causing stabilization of the system. These interactions are observed as increase in electron density (ED) in antibonding orbital that weakens the respective bonds of π bonds have a loftier density than the σ bonds, hence π→π* transitions have minimum delocalization energy than the σ→σ* transitions and bond of the ring (1.97e) evidently demonstrates strong delocalization. The bonding σ (C1-H12) and anti-bonding σ*(C4–C5) interactions results in a week stabilization energy of 0.55 kJ/mol.

Mulliken Population Analysis (MPA) and Natural Population Analysis (NPA): The Mulliken charges are the total and finest population analysis method. The electron population of each atom of the molecules is identifying, because of calculating the mulliken charges as explained by the density functional methods. The NPA is the finest and novelist method compare to the MPA method. Here NPA is the better while compare to the MPA because identified the NPA from NBO analysis. The MPA and NPA are obtained from optimized geometry and NBO results,

respectively. The both atomic charge calculation has an important role in the application of quantum chemical calculation to molecular system because of dipole moment, polarizability, atomic charge effect, electronic structure and a lot of properties of molecular systems. The calculated MPA and NPA atomic charges of 2C3MOBN are compared in Table 8. The two methods predict the equivalent propensities. The predicted atomic charges are explained through graphical representation (Fig.7). The polarization is the main theme of the charge changes in both population analysis methods. The charge distribution of the 2C3MOBN gives the Carbon charges had both signs in both methods. It has positive charge as well as negative with both population methods. Hydrogen atoms had net positive charge in both population methods, which denote the acceptor atoms. Oxygen and Nitrile atoms have negative charges both methods, which are donor atoms. The Oxygen atom had negative charge due to the positive charges of Hydrogen atoms. Chlorine atom had negative sign in MPA and positive sign in NPA. In overall comparison, Oxygen atom had highest electronegative charge (-0.543 e) in NPA method in the atom position.

Table.8. Comparison of Mulliken Population Analysis, Natural Population Analysis of 2C3MOBN

Atoms	6-311++G (2d, p)		Atoms	6-311++G (2d, p)	
	Mulliken	NPA		Mulliken	NPA
C1	-0.194751	-0.18483	C10	-0.696044	0.2853
O2	-0.346568	-0.54331	N11	-0.178775	-0.28824
C3	-0.32664	0.2962	H12	0.110409	0.15434
C4	0.027538	-0.22702	H13	0.151141	0.19053
C5	-0.084672	-0.18205	H14	0.141811	0.17006
C6	-0.442537	-0.1548	H15	0.125702	0.21325
C7	0.304291	-0.19439	H16	0.146748	0.21203
C8	1.131865	-0.03215	H17	0.149689	0.22077
C9	-0.019207	0.06432			

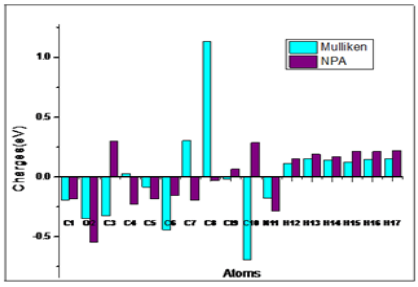

Figure.7. Mulliken and Natural Populations charges of 2C4MOBN

Additional Properties:

Thermodynamic Parameters: Several calculated thermodynamic parameters are given in Table.9. Scale factors have been recommended for an accurate predication in determining the zero-point vibration energies (ZPVE), and the entropy (S) vibration (T) and they can be used with the values of this table. On the other hand, the accurate prediction of Entropy, Enthalpy, Gibbs free energy, elevated heat energy and minimum energy had been calculated. The margin values of 2C3MOBN at room temperature at different methods, which gives the changes in the total entropy. The energies of whole molecules, the change in the total entropy and Self consistent field energy of 2C3MOBN at room temperature at different basic sets are also tabulated in Table.9.

Table.9. Thermodynamics parameters of 2C3MOBN.

Thermodynamic parameters Of DMAP	B3LYP
	6-311++G(2d,p)
Self-consistent field energy (a.u)	-898.749
Zero point vibrational energy (kcal/mol)	76.311
Rotational constant (GHz)	1.519
	0.810
	0.530
Rotational temperature (K)	0.073
	0.039
	0.025
Thermal energy (kcal/mol)	
Total	82.512
Translational	0.889
Rotational	0.889

Vibrational	80.734
Specific heat capacity at constant volume (cal/mol K)	
Total	36.205
Translational	2.981
Rotational	2.981
Vibrational	30.243
Dipole moment (Debye)	6.890
Entropy(S)(cal/mol K)	
Total	98.124
Translational	41.247
Rotational	30.578
Vibrational	26.299
Gibbs Free Energy	0.086
Enthalpy	-898.631
Thermal properties (Hartree/particle)	
Zero-point correction	0.121609
Thermal correction to energy	0.131491
Thermal correction to enthalpy	0.132435
Thermal correction to Gibbs free energy	0.085813
Sum of electronic and zero-point energies	-898.641589
Sum of electronic and thermal energies	-898.631707
Sum of electronic and thermal enthalpies	-898.630763
Sum of electronic and thermal free energies	-898.677385

Molecular Electrostatic Potential (MSP): The finest image exhibited technique to comprehend the comparative polarity of the particles is the MSP. A molecule has some space around them which produced at that point by the total charge distribution (negative charged particles + nuclei) of the molecule and correlates with the optical, electronic charges (anti positivity, partial) and organic reactivity of the molecule by the net electrostatic effect. This potential make over the electron density surface map portray the size, shape, charge density and reactive sites of the molecules. The electrostatic potential map shows the different colors that correspond to the different values of potentials like red and green be the negative and positive respectively. Finally blue represents the neutral potential. Potential decreases in the order blue > green > yellow > orange > red. The surface map, the contour plot and density of the title compounds are displayed in Fig.8a, 8b and 8c which are plotted using the computer software Gauss view.

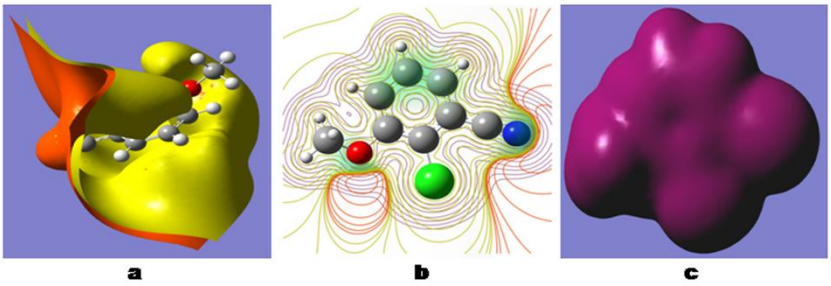

Figure.8. (a) The electrostatic potential (b) contour map and (c) electron density of 2C4MOBN

4. CONCLUSION

The computational DFT calculations are predicted the structural, optical, electrical and thermal properties of the title compounds. The equilibrium parameters, vibrational modes of assignments gives the fruitful correlative results while join with the observed values. The Electronic absorption and Frontier orbital transitions are calculated using the high basic set. NLO properties are predicted theoretically using the polar parameters of the molecules. These properties show that the title compound 2C3MOBN had good chemical stability, bioactivity and optics applications. From the NBO analysis identifies the molecule interactions, intra charge transformations which depend upon the structure of the molecules. The MEP surface map shows the comparative polarity. Ultimate calculated the thermal parameters of the compound. These results concluded the title compound is the best and good for all properties which helps to improve the future applications research and novel identifiers.

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