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Docking and Spectral Investigations on 2-Chloro-5-Nitropyridin-3-Carbonitrile by Quantum Computational Methods

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Abstract: In this work, structure of the molecule is analyzed in terms of molecular parameters like bond length, bond angleand dihedral angle calculated by Density Functional Theory Method(DFT) with B3LYP/6-311+G(d,P) and 6-311++G(d,p) basis sets. Non-Linear property of the molecule and Molecular electrostatic potential was studied. Atomic charge distribution of the title molecule has been investigated using the Mullikanatomic charge analysis. Stability of the molecule and charge delocalization has been studied by natural bond analysis.In this study discussed above docking analysis. Electronic transition in UV and HOMO-LUMO analysis.

Keywords: DFT; vibrational spectra; chemical shifts; HOMO-LUMO; Molecular docking

I. INTRODUCTION

Pyridine is a heterocyclic aromatic organic compound with a chemical formula C_5H_5N.The structure is related to benzene with one of its methine (=CH-) group replaced by a nitrogen atom. This nitrogen creates a tertiary amine which enables pyridine to undergo reactions such as alkylation and oxidation.

Amine presence in the ring causes a slight dipole on the ring which makes it unstable as compared to benzene. Many researchers are interested in pyridine and their derivatives because of its chemical properties and biological activity [1-2]. Pyridine is not available abundant in nature except in the leaves and roots of belladonnaand marshmallow[3].

Pyridine compound are volatile organic compounds in roasting process in fried chicken, potato chips, roasted coffee and fried bacon. Pyridine was isolated industrially from crude coal tar.

Today there are many methods in laboratory and in the industry for synthesis of pyridine and its derivatives. Their main commercial interest is in their conversion to other substances mainly drugs and dyes. Derivates of pyridine are commonly used as antihypersensitive, anti allergic, antitumor and analgesic agents.

Pyridine compounds substituted such as 2-halo-sustituted pyridine is an intermediate for preparing herbicides, insecticides and pharmaceutical.

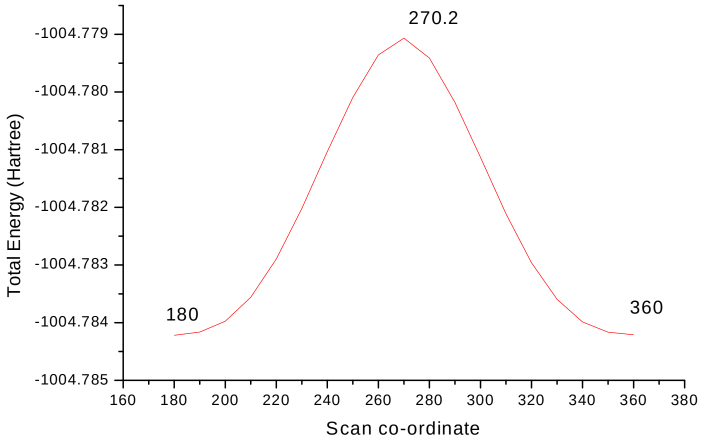
II. RESULT AND DISCUSION

A. *Conformational Analysis*

The conformational analysis of the molecule 2C5N3C was performed using B3LYP/6-311++G(d,p) method [4], by potential energy surface scan technique, by varying the dihedral angle C2-C1-O17-H18 in steps of 10^0 for a complete rotation $0-360^0$ [5].

The result of the scanning is shown graphically in Fig. 1 which clearly shows that there are two minimum at 0^0 and 360^0 with energy -0.1274 Hartree. Hence, these conformers both of them are structurally identical, serve as the most stable conformer of the compound.

There are two maximum energy points also at 59.42^0 and 308.57^0 with energy value -0.119 Hartree, which are the least stable conformers of the compound.



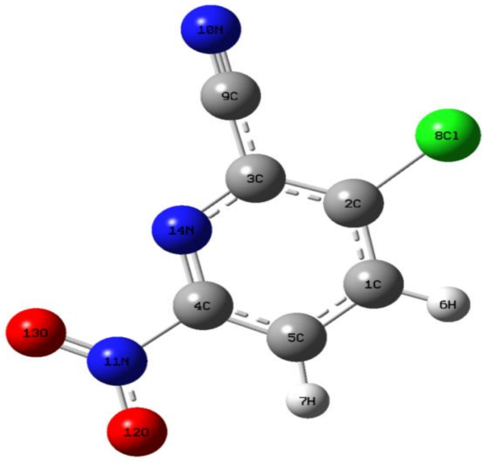


Fig. 1 Conformational Analysis

Fig. 2. Compound Structure in 2C5N3C

B. *Geometrical Analysis*

The bond distances are calculated by B3LYP/6-311+G(d,p) &6-311++G(d,p) method. The Optimized structure of 2C5N3C molecule was showed in Fig.2 and the structural parameters have been presented in Table 1. This molecule has four C-N, one C-Cl, two N-O, five C-C and two C-H bond lengths.The C-C bonds, C-N bonds, C-Cl bond, and N-O bonds in the main frame of Pyridine rings are usually ranged between 1.345-1.433 Å, 1.329-1.344 Å, 1.73-1.75Å and 1.38-1.39 Å respectively [6]. Here, the C-C bond lengths were observed to be 1.38–1.43Å values are in between the expected range and C-N bond lengths were appeared to be 1.15-1.50 Å respectively. The impact of substitution on ring was pronounced by the slightly change of C-N values. The optimized C-Cl bond length is 1.73Å and C-H bond length are1.08Å values equal in expected range. Inter molecular bond lengths between nitro and chloro groups were observed symmetrically. C-C-C bond angles values are expected around 120 Å [7] in present molecules are all in expected range but C1-C5-C4 is 116 Å values in lowest range is due to the any substance is not present of the molecules. In C-C-H bond angles are also equal in expected range and C5-C4-N14 bond angles is 125 Å values is higher than the expected range is due to the presence of carbonitrile group but all other values are lies in the expected range. All the values are expected in XRD range [7].

Table 1 Structural parameters of 2-chloro-5-nitropyridine-3-carbonitrile

Structural Parameters	B3LYP / 6–311+ G(d,p)	B3LYP / 6–311++ G(d,p)	XRD	Structural Parameters	B3LYP / 6–311+ G(d,p)	B3LYP / 6–311++ G(d,p)	XRD
Bond Length				Bond Angle			
C1-C2	1.3926	1.3934	1.398	C2-C1-C5	119.0503	119.0502	115.89
C1-C5	1.3835	1.3875	1.375	C2-C1-H6	119.9226	119.9134	119.20
C1-H6	1.0822	1.0825	1.081	C5-C1-H6	121.0271	121.0364	118.22
C2-C3	1.4026	1.4076	1.393	C1-C2-C3	118.8508	118.8519	118.22
C2-CI8	1.7322	1.7322	1.720	C1-C2-CI8	120.1385	120.1306	119.01
C3-C9	1.4363	1.4363	1.433	C3-C2-CI8	121.0107	121.0175	191.11
C3-N14	1.3362	1.3367	1.313	C2-C3-C9	121.2893	121.2901	120.07
C4-C5	1.3911	1.3918	1.389	C2-C3-N14	121.7645	121.7625	120.02
C4-N11	1.5073	1.5076	1.476	C9-C3-N14	116.9462	116.9474	115.71
C4-N14	1.3893	1.3097	1.332	C5-C4-N11	118.6769	118.6745	117.01
C5-H7	1.0801	1.0805	1.080	C5-C4-N14	125.5759	125.5754	120.40
C9-N10	1.1536	1.1535	1.135	N11-C4-N14	115.7472	115.7501	111.24
N11-O12	1.2219	1.2259	1.212	C1-C5-C4	116.8072	116.8075	122.06
N11-O13	1.2113	1.2116	1.213	C1-C5-N7	122.3488	122.3461	122.33
				C4-C5-H7	120.8439	120.8464	121.08

C. Mullikan And Natural Atomic Charge Analysis

Charges calculations have an important role as the atomic charges cause the dipole moment, molecular polarizability, electronic structure and molecular reactivity of the system [8]. The charges on the atoms of the present compound are calculated by Mullikan and natural charge analysis using B3LYP method with 6-311++G(d,p) basis set, the graphical representation of the results are presented in Fig3 and Table 2. In this ring all the carbon atoms C1 is found to be negative in both atomic charges. Then C4 and C9 are highly negative in Mullikan charge due to the presence of neighboring nitrogen atom and Positive in Natural charge. As C3 atoms is a show to be positive in both atomic chare. Then C2 and C3 atoms are almost equally positive in Mullikan charge analysis is due to the presence of Cl 8 and N14 atom. In case hydrogen atoms are positive in both charges. The nitrogen atom have N10 is both negative and N11 is negative for Mullikan positive in natural and N14 is positive for Mullikan and negative in natural charge analysis. O12 is negative in both charges. Then O13 is positive in Mullikan and negative in natural atomic charge. Similarly the Cl atom is attached to pyridine ring expected to be positive because it repulsive it is found to be positive in both charges.

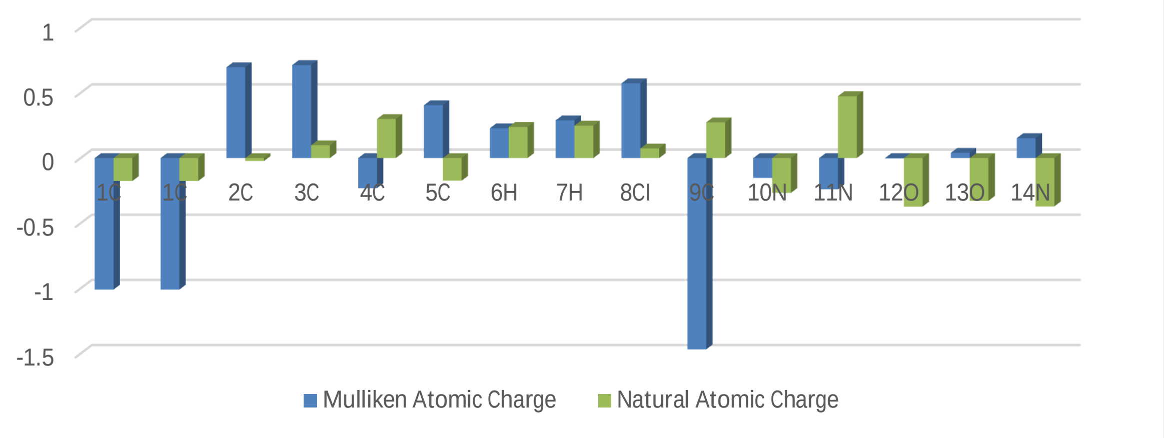


Fig. 3 Charge analysis

Table 2Mulliken charges of 2-chioro-5-nitropyridine-3- carbonitrile with B3LYP/6-311++G(d,p)

Atoms	2-chioro-5-nitropyridine-3- carbonitrile	
	Mullikan Atomic charges	Natural Atomic charges
1C	-1.00906	-0.17616
2C	0.696621	-0.02219
3C	0.713729	0.09825
4C	-0.23046	0.29965
5C	0.405719	-0.17369
6H	0.228895	0.2391
7H	0.289463	0.24911
8CI	0.573883	0.07391
9C	-1.46732	0.27408
10N	-0.15267	-0.26709
11N	-0.23975	0.47514
12O	-0.00229	-0.372
13O	0.04035	-0.32749
14N	0.152889	-0.37061

D. NMR spectra and Calculations

The stimulated proton and carbon chemical shift of the experimental molecule 2C5N3C have been compared with the experimental data [9] as shown in Fig 4 and table 3. Chemical shifts are reported in ppm relative to TMS for ^{1}H and ^{13}C NMR spectra. The geometry optimization of the 2C5N3C was performed at the gradient corrected density functional level of theory using the hybrid B3LYP method based on Becke's three parameters functional of DFT. Then, gauge – including atomic orbital (GIAO) ^{13}C NMR chemical shift calculations of the compound was made by the same method using 6-311++G (d,p) basis set IEFPCM/$CDCl_3$ solution.

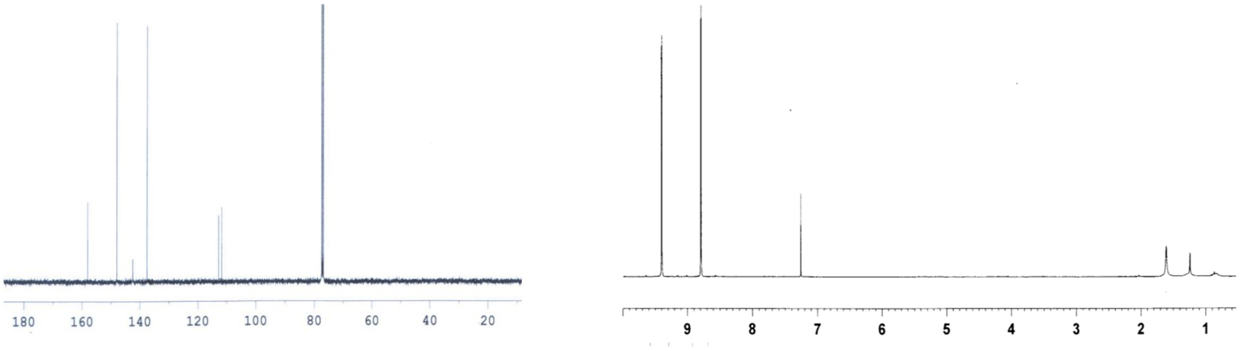


Fig.4 C and H NMR Experimental Analysis

Aromatic carbons give signals in overlapped areas of the spectrum with chemical shift values from 120 to 130 ppm. In our present investigation, the experimental chemical shift values of aromatic carbons are in the range 111.8– 158.0 ppm. The N and O atoms more electronegative property polarizes the electron distribution in their bonds to adjacent carbon atoms C4 (158.0ppm) and increasing the chemical shift value. On the basis of ^{13}C NMR spectra, the ring carbon C2 (147.9 ppm) is higher chemical shift than the other carbon atoms due to the presence of chlorine atom. The chemical shift value of C1(142.4 ppm) is higher than the other aromatic carbons because of the substitution of pyridine group. The C9 (111.8 ppm) is lesser than the aromatic carbons range due to the attached in triple bonded nitrogen. The computed chemical shift value for pyridine group carbon atom is in good agreement with the measured values. The studied molecule has hydrogen atoms attached to the ring, pyridine group. The chemical shifts obtained and calculated for the ^{1}H atoms are experimentally observed at 7.31 and 8.70 ppm, respectively. The 7H atoms are good agreement with the computational values. And 6H atoms are slightly low because the atom is placed edges of the ring.

Table 3Calculated ^{1}H and ^{13} C NMR chemical shifts (ppm) of 2-chloro-5-nitropyridine-3-carbonitrilewith B3LYP/6-311+G(d,p)

Atoms	Theoretical		Experimental $CDCl_3$
	Gas	$CDCl_3$	
	B3LYP/6311++G(2d,p) (ppm)	B3LYP/6311++G(2d,p) (ppm)	
1C	144.785	147.342	142.48
2C	156.225	158.511	147.90
3C	136.258	134.616	137.56
4C	159.964	160.506	158.09
5C	125.039	127.65	112.84
9C	116.923	118.837	111.82
6H	7.9272	8.2472	7.31
7H	8.4671	8.6719	8.70

E. Vibrational Analysis

The maximum number of potentially active observable fundamentals of a non-linear molecule which contains N atoms is equal to (3N – 6) apart from three translational and three rotational degrees of freedom. Hence 2C5N3C molecule that is planar has 14 atoms with 36 normal modes of vibrations. The observed and stimulated infrared and Raman spectra of 2C5N3C is shown in Figs 5 respectively. The observed and scaled theoretical frequencies using DFT (B3LYP) with 6-311++G (d, p) basis sets with TEDs are listed in Table 4.

F. C-H vibrations

The aromatic C-H stretching vibrations in tetra substituted benzene rings are generally observed in the region 3000 – 3100 cm^{-1} [10]. In this compound are experimentally observed at 3101 & 3088cm^{-1} in FT-IR and 3066 cm^{-1} in FT-Raman respectively. The bands due to C-H in plane bending vibrations are observed in the region 1000-1300 cm^{-1}[11] for observed at 1135 & 1130 cm^{-1} in FT-IR and at 1113& 1110cm^{-1} in FT-Raman. The C-H out-of-plane bending vibrations appear within the region 900-675 cm^{-1} [11]. The vibrations are identified at 955, 937 &862 cm^{-1} in FT-IR and FT-Raman are in good agreement with the experimental values and literature.

G. Ring Vibrations

The ring stretching vibrations are expected within the region 1620-1390 cm^{-1}[12]. Most of the ring modes are altered by the substitution to aromatic ring. The C-C vibrations in the ring are observed at 1514, 1390 &1360 cm^{-1} in FT-IR and 1518 &1511 in FT-Raman. All bands are observed in the expected range. The infrared bands at 703, 628 & 579 cm^{-1} in FT-IR and 695, 665, 603 & 559 cm^{-1} inFT-Raman in-plane bending & out-of-plane vibrations of 2C5N3C. The calculated scaled values are 713, 673cm^{-1}.

H. C-N, O-N and C-O vibrations

The C-N stretching frequency is a rather difficult task since there are problems determinations of these frequencies from other vibrations. The C-N stretching absorptions are observed in the region 1382-1266 cm^{-1} for aromatic compound [13]. In the present work, the band at1577 cm^{-1} in FT-IR and at1575 &1518 cm^{-1} FT-Raman spectrum is assigned to C-N stretching vibration. The N-O Vibrations at 1303 cm^{-1} in FT- Raman. In this compound C-Cl bending vibration is experimental at 1011 cm^{-1} in FT-Raman and Observed at 1063 cm^{-1}. The C-Cl Torsion vibration is 522 & cm^{-1} in FT-IR and Raman and Observed 520 cm^{-1}.

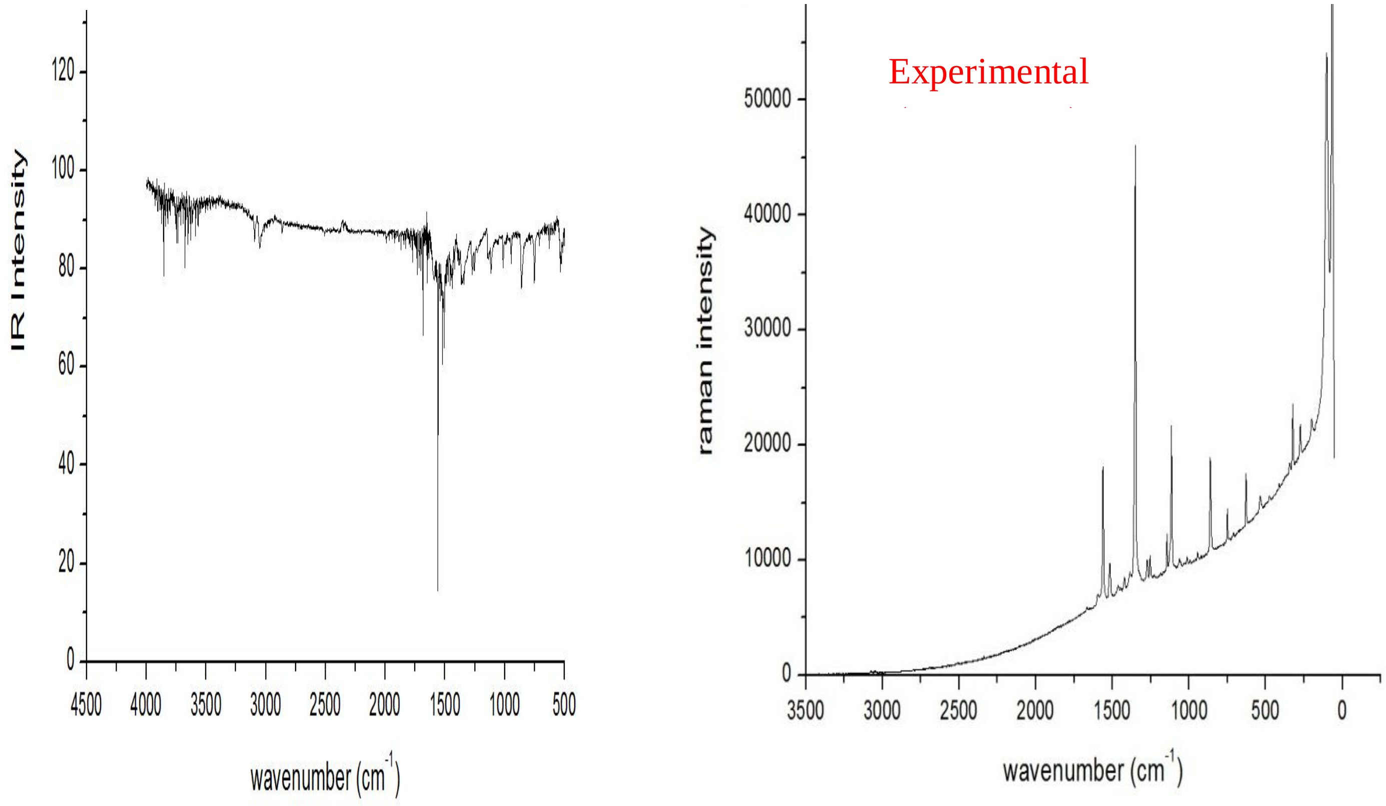


Fig. 5 Experimental FT-IR & FT-Raman Spectrum

Table: 4 The Observed FT-IR and FT-RAMAN Calculated frequencies using B3LYP-6-311G(d,p) basis sets of 2-Choloro-5-Nitropyridine-3-Carbonitrile

Symmetry species cm^{-1}	Experimental Wavenumber (cm^{-1})		Calculated Wavenumber (cm^{-1})		Assignment	VED
	FTIR	FT-RAMAN	Un scaled	Scaled		
A’	3101		3234	3105	υC-H	υCH 96
A’	3088	3066	3207	3078	υ C-H	υCH 96
A’	2250	2243	2352	2258	υC≅N	υCN 89
A’	1577	1575	1644	1578	υC≅N	υON 34 +υNC 12
A’		1518	1605	1541	υ C=C	υ ON 21 + υNC 19
A’	1514	1511	1581	1517	υ C=C	υ CC 32 + υ HCC 11
A’	1390		1446	1388	υC-C	υCC 14 + β HCC 29 + β HCC 21
A’	1360	1358	1422	1365	υC-C	υCC 10 + υ NC 29
A’		1303	1370	1316	υN-O	υ ON 49
A’	1250		1306	1254	υ C-N	υ NC 29
A’		1172	1227	1178	υC-C	υ CC 18 + β HCC 13
A’	1135	1130	1173	1126	β C-H	υCC + υ NC 10 + β HCC 31
A’	1113	1110	1150	1104	β C-H	υ CC 21 + β HCC 51
A’	1011		1063	1020	ν C- C1	ν NC 11 + ν C1C 15
A’’	955	937	1000	960	ν C-H	τ HCCH 92
A’	862		920	883	ν C-N	ν NC 13
A’’		809	867	833	ν C-N	τ NCCC 83
A’	786	781	818	785	β N=O	β CCC 12 + β ONO 52
A’’	747	737	770	740	β N-O	ν OCON 57 + τ CNCN 12
A’	703	695	743	713	ν C-C	τ CCNC 57 + τ CCCC 52
A’		665	702	673	ν C-C	β CCC 12 + β CCN 24
A’	628	603	643	617	ν C-C	β CCC 33
A’’	579	559	597	573	ν C-C	τ CCCN 15 + τ CCCC 10
A’	522	511	542	520	β C-C1	β CCC1 10 + ν C1C 18
A’	500	492	518	497	β C-N	β CNO 50
A’’		459	481	462	β C-N	τ CCCN 21 + τ CCCC 43
A’		433	445	428	β C-N	β CCC24 + β CCN 10 + ν NC 13
A’’		373	394	378	ν C-N	τ CCCN 42 + τ CCNC 26
A’		320	317	305	ν C-N	β CCN 18 + β CNO 16
A’		315	315	302	ν C-C1	ν NC 30 + ν C1C 17 + β CCC 16
A’’		275	282	270	β CCC	τ CCCC1 52
A’		179	188	180	β CCC	β CNO 10 + β CCC1 35
A’’		130	138	133	β NCC	τ CNCN 16
A’		94	128	123	ν NCC	β CCC 44 + β CCN 14
A’’		63	80	76	ν CCC	τ CCCC 13 + τ CCCC1 34
A’’		60	24	23	ν CCC	τ CCNO 93

I. UV-Visible & Homo-Lumo Analysis

The UV-Visible band is consists of entire energy transitions among vibrational energy levels. Normally, the parameters of 2C5N3Care computed using B3LYP with function and 6-311++G (d,p) basis set along with TD–SCF method. The experimental and calculations are performed for $CdCl_3$ solvent phases [16]. The excitation energies, oscillator strength (f) and absorption wavelength (λ) and HOMO–LUMO contributions are presented in Table 5. The UV- theoretical andExperimental spectra are presented in

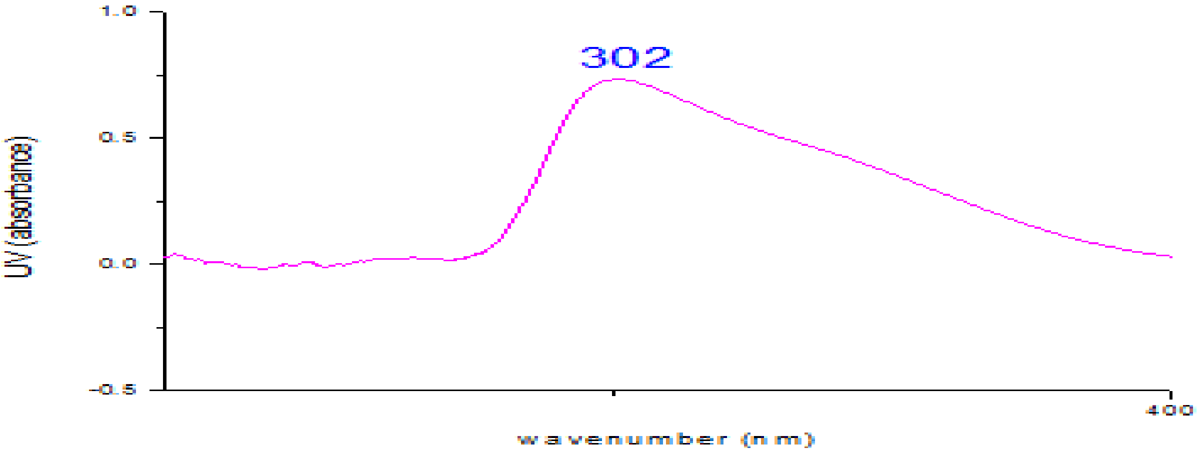


Fig. 6 Experimental UV spectra

Fig.6. In this case, the electronic absorption bands on the energy gap of 3.6, 4.1, 4.6 eVand their absorption wavelengths are 338, 302, 226 nm was identified respectively with the maximum oscillator strength 0.0012. In solvent phase, the band was found at 329, 295, 287 nm with the energy gap of 3.7, 4.1, 4.3 ev respectively. The strength of oscillations was measured as 0.2424 and is represented by n→π* (302nm) and also all the bands were taking place in Quartz UV region of the spectrum.

Table 5 Theoretical electronic absorption spectra of 2-chloro-5-nitropyridine-3-carbonitrile

λ (nm)		E(eV)	(f)	Major contribution
Theo. (Gas)	Exp.			
338.81		3.6594	0.0000	H-1->LUMO (87%), H-2->LUMO (7%), H-1->L+2 (4%)
302.39		4.1001	0.0000	H-2->LUMO (83%), H-5->LUMO (8%), H-2->L+2 (3%)
266.95		4.6445	0.0012	H-2->L+1 (12%), H-1->L+1 (76%), H-5->LUMO (3%)
Cdcl3				
329.57		3.7620	0.0000	H-3->LUMO (15%),H-1->LUMO (78%), H-4->LUMO (2%)
295.92	302.3	4.1898	0.0000	H-4->LUMO (15%), H-3->LUMO (71%), H-1->LUMO (10%)
287.84		4.3074	0.2424	HOMO->LUMO (92%), HOMO->L+1 (3%)

The HOMO-LUMO energy gap and different reactivity descriptors [17] of molecule in both levels are presented in Fig 7 and Table 8. The calculated energy of the HOMO is -0.313 eV and that of LUMO is -0.161eV. The energy gap between is -0.152eV,which shows the possibility of flow of energy from HOMO to LUMO.

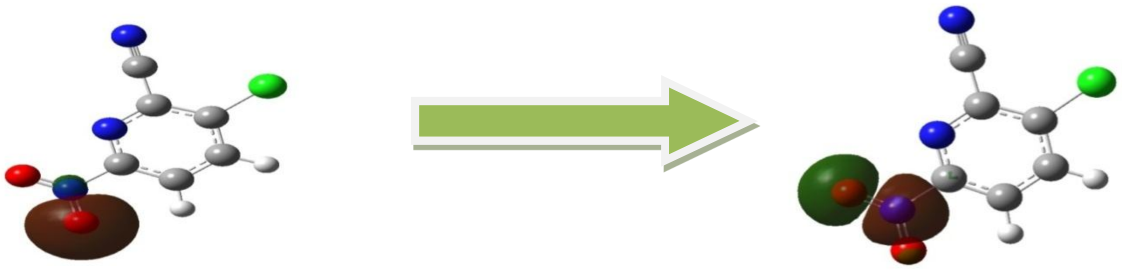


Fig.8. HOMO - LUMO

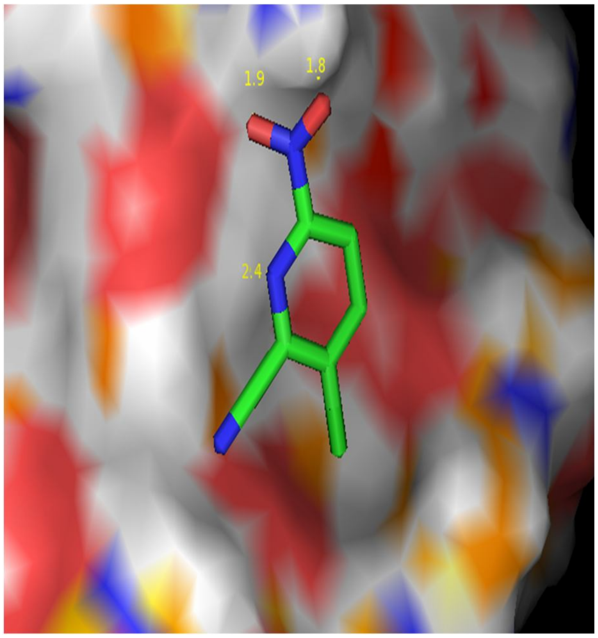
Table7 HOMO, LUMO 2-chloro-5-nitropyridine-3-carbonitrile

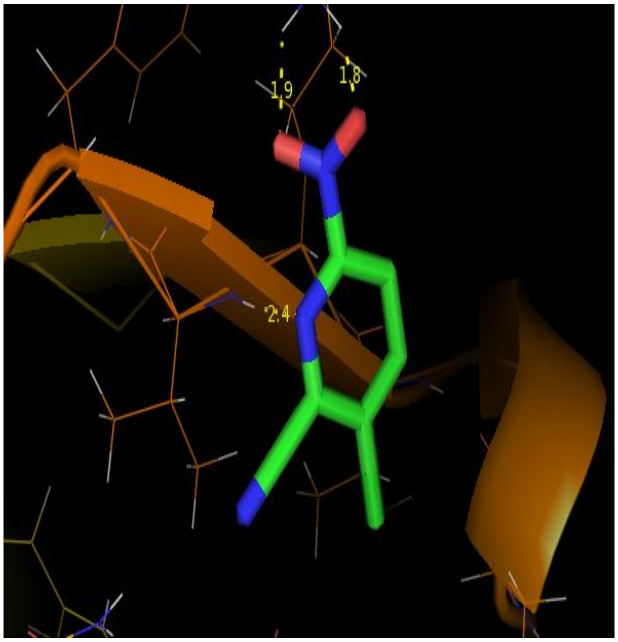
Parameters	2-chloro-5-nitropyridine-3-carbonitrile
E_{HOMO} (eV)	0.31348
E_{LUMO} (eV)	0.16142
$\Delta E_{HOMO\text{-}LUMO\ gap}$ (eV)	0.15206
Electronegativity (χ) (eV)	-0.23745
Chemical hardness (η) (eV)	-0.07603
Global softness (σ) (eV)	-0.30412
Electrophilicity index (ω) (eV)	-0.37077

J. Docking Study

The structures of the molecule can prediction of activity spectra using pass online. For docking study high resolution fine crystal structure of (PDB ID 2CUT).To investigate the binding affinity of drug within the so many target protein was used Auto Dock program 4.0 [19]. On the basis structure of molecular spectra is Prediction of Activity Spectra (PASS) [20] due to online tools for various activities. The active site to the energies was defined to add residues of active side with the use of grid size Å 80 Å 80 Å. The Binding Energy (Kcal/mol) was calculated. In this fig yellow dotted lined denote the formation of hydrogen bond of ligand with target proteins is also illustrated using pymol software. Hydrogen bond length of 1.8, 1.9 and 2.4 Å shows the existence of the ligand-protein interaction.

Protein (PDB ID)	No. of hydrogen bond	Bonded Residues	Bond Distance
2CUT	3	LYS168	1.8
		LYS168	1.9
		VAL169	2.4





III. CONCLUSION

The optimized structural parameter such as bond length, bond angle and dihedral angles are calculated at DFT/B3LYP/6-311++G(d,p) method and also compared with reported XRD values. The conjugative systems possess more Non-linear optical behavior, evident from first order hyper polarizabilities. NBO analysis reflects the charge transfer occur within the molecule. The Lewis and non-Lewis structure of 2C5N3C shows that the contribution of ED of individual atoms, which leads the molecular vibration with respect to hybridization of chemical bonds. HOMO and LUMO orbitals have been visualized. The MEP map shows the negative potential sites on oxygen and nitrogen atoms as well as the positive potential sites around the hydrogen atoms. Finally, the complete vibrational assignments of 2C5N3C analyzed with the help of TED contribution. The electronic features,such as absorption wavelength (λ), excitation energies (E), and oscillator strengths (f) have been investigated by experimental and theoretical methods.

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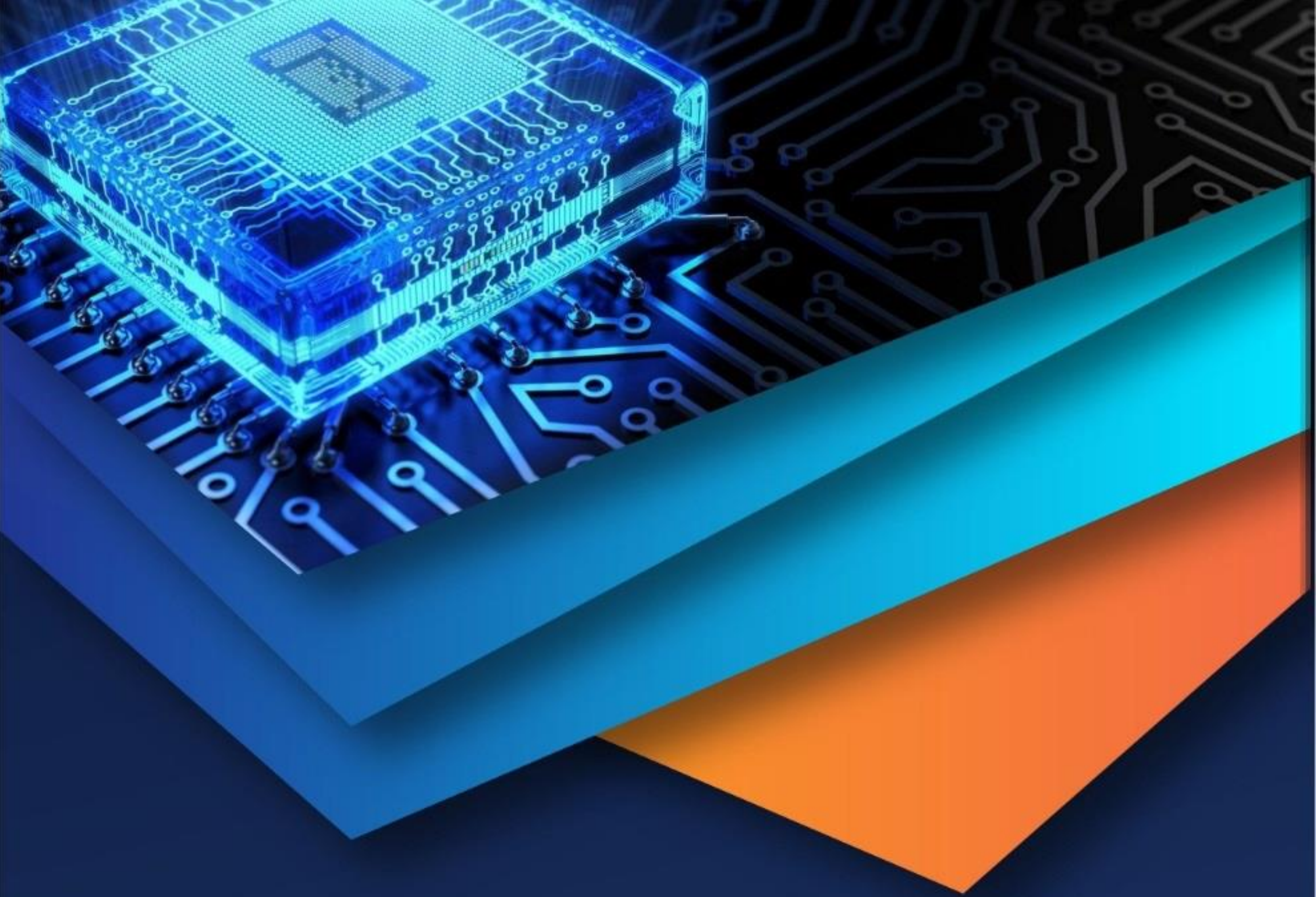

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