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Experimental and Theoretical Vibrational Spectral Study of 4,5-Difloro-2-nitroaniline

[1]Vishrut Chaudhary

[1]Department of Chemistry, Deva Nagri College, Meerut-250002, U.P., India

[1]ch.vishrut2012@gmail.com

ABSTRACT

In the present work, the optimized structure of the 4,5-Difloro-2-nitroaniline have been calculated. The vibrational analysis has carried out experimentally and theoretically. The effect of amino and nitro group substitution in benzene ring has been analysed by Hartree-Fock (HF) and time-dependent density functional theory (TD-DFT). In the present work a comparative detail between the observed fundamental vibration frequency/wavenumber of the title compound given with the calculated harmonic vibrational wavenumber at B3LYPand HF.

Keywords: 4,5-Difloro-2-nitroaniline, Vibrational analysis, Hartree-Fock, Density functional theory.

1. INTRODUCTION

Aniline and its derivatives have been subjected to many different types of scientific studies up to now. Aniline is six membered homoaromatic simplest amine containing – NH2 functional group. Aniline has significant industrially commodity chemical and also use for fine chemical synthesis. Due to having electron rich benzene ring aniline goes to electrophilic aromatic substitution. After formation of diazonium salt through diazotization reaction this diazonium salt goes to a huge number of nucleophile substitution and form a lot number of compounds used in daily life. They have been broadly used for pharmaceutical manufacturing, electro-optical, chemical dye industries and for other commercial and industrial use, and have been studied extensively [1-3].

Some para substituted compounds of aniline are frequently used local anaesthetics. Among these compounds the amino group plays crucial role in the interaction with the receptor. Therefore, studies of properties as well as the extensive experimental nature of reaction mechanics, [4] and theoretical investigations of substituted aniline have focused on determine the structure and vibrational assignments of aniline and its methyl derivatives [1-8]. Molecular geometry alters due to enhanced interaction between the aromatic ring and the amino group. Substituent group inclusion in aniline also explains the change of charge distribution with in the molecule [9-13]. “It’sgeometry has been reported using semi-empirical [14-15], ab-initio methods [14,16-17]. Extensive recent studies on vibrational spectra of substituted anilines assigned [1,5,8,18-20] complete vibrational mode and frequency analyses. Assignment of some bands observed in the infrared spectrum of p-methylaniline are given in literature [4,21-25]. Vibrational modes and frequency analyses of m-methylaniline have been studied by Alutun et al. [1]. The vibrational spectra of

fluoromethylaniline [26-27] and chloromethylaniline have been reported. Shanker et al. [28] studied 2-chloro-6-methylaniline with polarized Raman and infrared spectra" [29].

Vibrational assignment-based F.T.I.R analysis in solution and liquid phase the vibrational spectral and first order hyperpolarizability of N-Phenylbenzenesulfonamide and 2,5 diflouronitrobezene have been calculated [31-32]. Spectral analysis and bioactivity of 4-Chloro - 3-ferrocylaniline, 2,5,6 -trichloroaniline and 2,5 diflouroaniline have been investigated by DFT and NMR and electronic spectroscopes [33-37].

Spectroscopical and DFT studies were also reported of 3 methoxyaniline by Sivasanjini et al [38] and 3,4-diflouroaniline by Kose et al. [39]. The FTIR and FT-Raman of 4-(4-aminobenzene) suflonyl aniline has been recorded and analyzed. The equilibrium geometry, harmonic vibrational frequencies have been investigated with the help of HF and DFT methods. 4- chloro - 2-flouroaniline and 4 - chloro-N-methylanilineexperimentally observed spectral data (FT- IR and FT- Raman) was compared with the spectral data obtained by DFT method. The theoretically constructed FT-IR and FT- Raman spectra exactly coincide with experimental one. The experimental and the retical study on the molecular structure and vibrational spectra of 2,4,5 - trichloroaniline were studied. The FT - IR and FT-Raman spectra were recorded and also calculated by DFT [40-43]. 3- (triflouromethyl) aniline was studied theoretically by DFT and experimentally by Arjunan et al. [44-46].

2. EXPERIMENTAL DETAILS

The investigated compound 4,5-Difloro-2-nitroaniline (4,5DF2NA) was purchased from Tokyo chemical (TCI) India Pvt. Ltd with stated purity of more than 99.9% and was used as such to record FT-Raman spectra without further purification. The FT-IR absorption spectrum of 4,5DF2NA was recorded in central Instrumentation Facility, Jamia Millia Islamia, New Delhi on Bruker, Tensor 37 range 4000-600cm-1. The Raman Spectrum was recorded in the range of 3500-100cm-1 in the Centre for nanotechnology.

3. COMPUTATIONAL DETAILS

In the present work after getting the data and spectrum recorded by experimentally by different spectrophotometer of the compound 4,5-Difloro-2-nitroaniline the theoretical calculations are carried out. Two different methods are applied for these calculations, Hartree -Fock (HF) and density functional Theory (DFT). For making structure and visualize the geometry the Gauss view molecular visualization program was run while for the calculations of vibrational geometrical, electronic and thermodynamic parameters Gaussian-09 program [47] set was employed. Three parameters that are combined with DFT by Lee, Yang and Parr (LYP) is electron correlation functional [48]. These three-hybrid functional group (B3) parameters by Becke's [49] were used for DFT calculations make one single election density functional method B3LYP. In this work two different theory HF and B3LYP with same basis sets, 6-311++ (d,p) are used for the titled compound.Basis sets are very important in these quantum calculations. Baris sets are groups of wave functions for orbitals of the molecules, be it is the possibility to change in size of these orbitals the by the multiple split valence wave function.After optimized the structure title compound at the two different basis set by the two empirical quantum chemical theory, Hartree-Fock and density functional theory, the bond

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length, dihedral angle and bond angle was calculated. Vibrational frequencies (IR and FT-Raman) were also calculated with help of these two theories and obtained the spectrum of the 4,5DF2NA. These unscaled frequencies are multiplied by scaling factor to get the scaled frequencies for 4,5DF2NA. Potential energy distribution (PED) and vibrational assignments also calculated by density functional theory at B3LYP/6-311 by the VEDA-4. For making this study more authentic, results, obtained by HF and DFT compared with the results obtained by experimentally.

4. RESULT AND DISCUSSION

4.1 Molecular Geometry

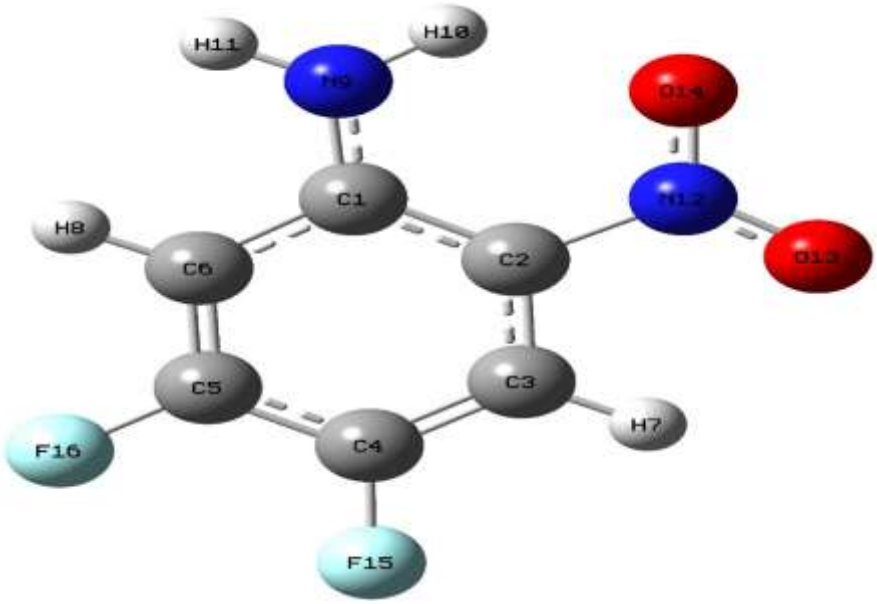

Figure 4.1 Optimized geometric structure of 4,5-Difloro-2-nitroaniline with numbering of atoms.

The structure and scheme with number of atoms of the compound 4,5-difluoro -2-nitro aniline was explained in the present study. For the geometrical demonstration of the title compound, Cs point group symmetry has been taken account for this. In this research study Cartesian coordinate analysis of theoretical force constant took into consideration. The computation have been started with 168 symmetry adapted basis functions ,168 symmetry adapted Cartesian basis functions ,332 primitive gaussians ,for 44 alpha and 44 beta electrons with nuclear repulsion energy ;686.6262 Hartree assuming Cs point group symmetry of the optimized structure of title compound .To find out the optimized structure, conformation and orientation of -NO2 and F atom in aniline molecule polarised set 6-31++G(d,p) and 6-3111++G(d,p) are used in this investigation .

4.2 Vibrational Analysis

For the vibrational analysis of 4,5DF2NA, calculations were performed with help of HF and DFT models. Both F group and NO2 group are deactivating group which decrease electron density from aromatic nucleus, while NH2 group activate the ring by donating resonance effect. In liquid phase this molecule gives strong H-bond interaction and F-F Interaction.

C-H Vibration: In this homoaromatic molecule two isolated C-H stretching vibration present. In present work large difference arises due to the adjacent group NO2 and NH2. The presence of N-N and C-H stretching vibration in homoaromatic structure shown above 3000cm-1 that is used as a ready reckoner for the identification of structure due to characteristics region [41]. IR vibration observed frequency obtained peak at 2356 cm-1and calculated by HF lies 3182-3217cm-1. Observed Raman vibration is of very weak intensity and appear at 3345 cm-1 while calculated value for the same vibration lies between 3146-3180cm-1. H bonding play important role for this deviation in liquid phase.

C-C Vibration: - In the title molecule aromatic nucleus have six ring stretching vibration in which υC3-C4(11) and υC5-C4(29) sym. stretching while υC6-C5-C4 and υC-C6-C5 in plane bending vibration the observed IR frequency of weak intensity obtained at 1648 cm-1 while Raman observed vibration obtained at 1572cm-1. On HF scaled IR vibration obtained at 1650 cm-1 while on DFT scaled 1577cm-1.These vibrations are substituent sensitive and it's not easy to differentiate with other mode of vibration.

C-F Vibration: - Calculation of C-F stretching modes are very difficult because of these vibrations are strongly coupled with the other in plane bending vibrations. The observed band of the C-F stretching vibration have been found in Raman of medium intensity is 875 cm-1. C-F stretching vibrations strongly coupled with the C-H in plane bending vibrations of βC1C6C5 and out of plane bending of γO14C2O13N12 (12). The calculated frequency through HF 877cm-1 and by DFT calculation it found at 834 cm-1. The intensity of υC4-F14(18) are found 45.31 in IR and 40.93 in Raman spectral analysis. All the C-F vibration are not found in expected region this is due to substituent sensitive effect.

C-N Vibration: The C-N stretching vibration usually lies in the region 1400-1200cm-1 for aromatic compound. The assignment of C-N vibration is rather difficult task since the mixing of vibration is possible in this region explain by Silverstein et. al. [21,41]. In this spectral analysis the band observed at 1163cm-1 on HF and 1068 through DFT. This is due to the coupling of C-N bond with C-F bond. The in plane and out of plane bending C-N vibration have also been identified. These assignments are also supported by the frequencies calculated by DFT.

NO2-Groupvibration: Molecule having the NO2 group the NO2asymmetric stretching vibration band range is 1625-1540 cm-1 and that of symmetric stretching vibration is 1400 – 1360 cm-1. In Title molecule 4,5DF2NA observed Raman frequency is 790cm-1. It appears at 803cm-1 in HF and at 771cm-1 DFT calculation. The deformation vibrations of NO2 group like rocking, wagging and twisting contribute to many common vibrational modes of low intensity. We also know that torsion vibration is very enharmonic, its frequency is difficult to regenerate with the opposite approach.

NH2-Group vibrational Analysis: - Varasanyi [24,50] reported that NH2 group show six internal modes of vibration like, symmetric stretching at lower IR frequency, asymmetric stretching at higher frequency 3500-3300cm-1and the antisymmetric plane deformation or rocking (βas) at 1590cm-1. The NH2 stretching vibration show shift in higher frequency in the title molecule due to the presence of strong -I Group like F and NO2. They also

dominantly show mesomeric effect at ortho and para position. In present study it is observed that asymmetric stretching of - NH2 group observed at 3745 cm-1 and 3639 cm-1 using by HF and DFT methods respectively. This is due to strong electron attracting substituents at meta position. This results good agreements with the experimental value at 3740 cm-1 of strong intensity. Experimental IR symmetric stretching is very weak in intensity and observed at 3628cm-1 and calculated value from HF and DFT calculation it is observed on are 3611cm-1 and 3477cm-1 respectively.

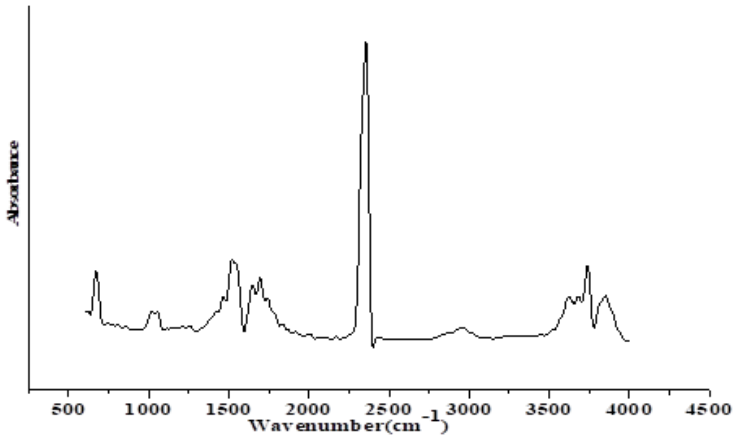

Fig 4.2(a): Experimental FT-IR spectra of 4,5-Difloro-2-nitroaniline

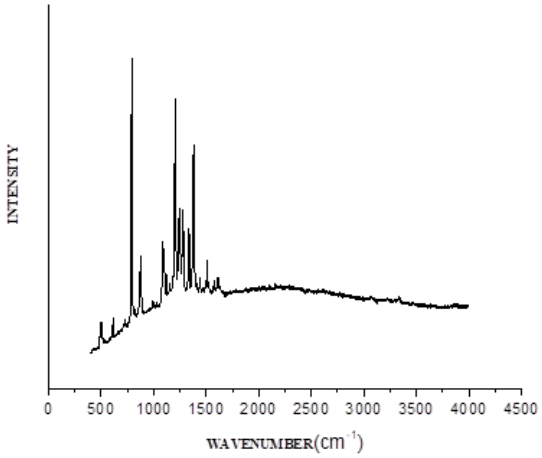

Fig 4.2(b): Experimental FT-RAMAN spectra of 4,5-Difloro-2-nitroaniline

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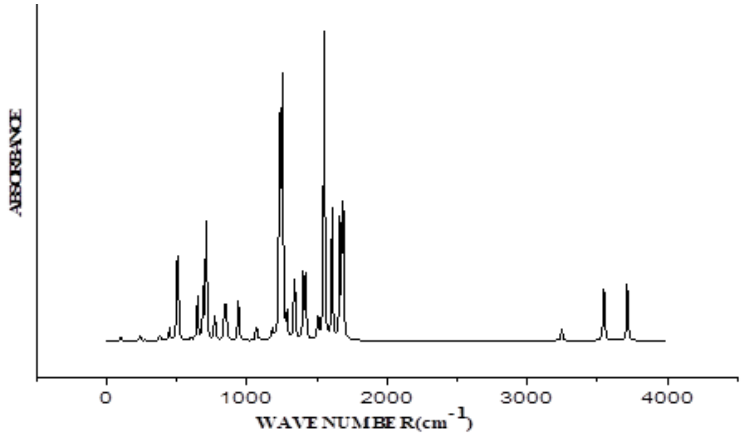

Fig 4.2(c): Calculated FT-IR spectra of 4,5-Difloro-2-nitroaniline with B3LYP/6-311++G(d,p)

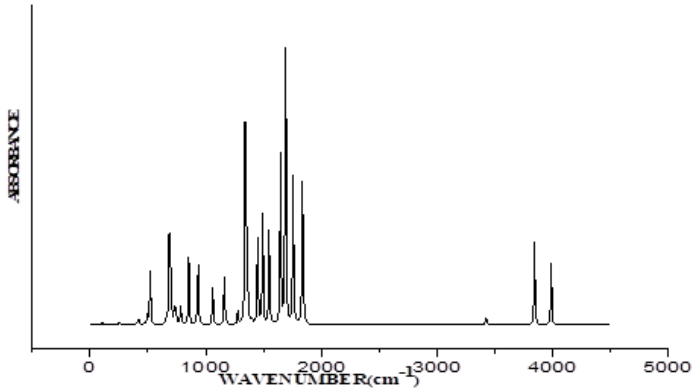

Fig 4.2(d): Calculated FT-IR spectra of 4,5-Difloro-2-nitroaniline with HF/6-311++G(d,p)

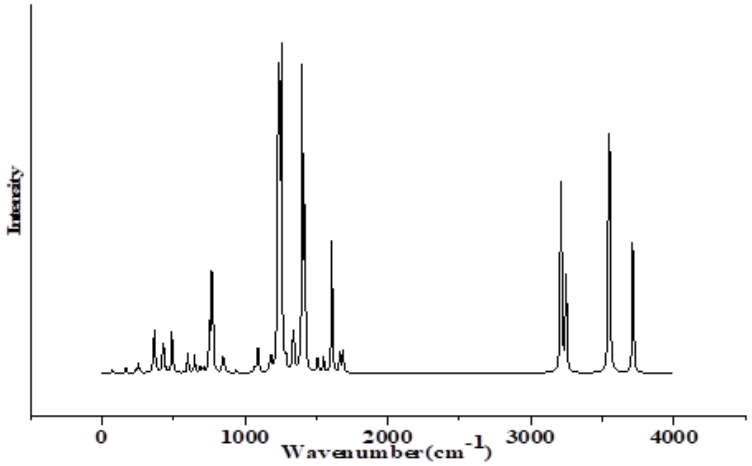

Fig 4.2(e): Calculated FT-RAMAN spectra of 4,5-Difloro-2-nitroaniline with B3LYP/6-311++G(d,p)

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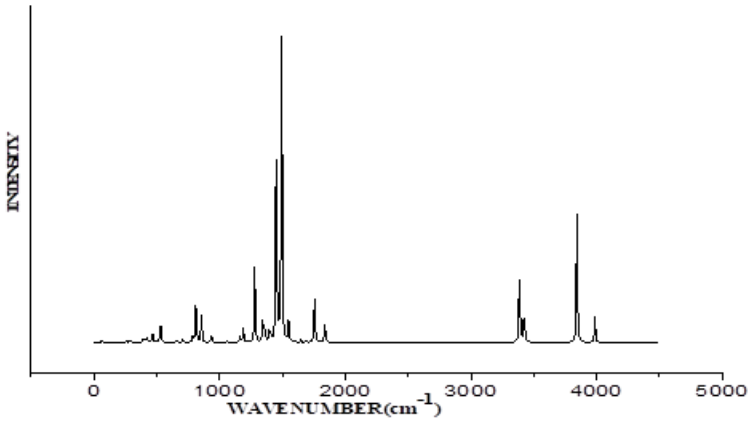

Fig 4.2(f): Calculated FT-RAMAN spectra of 4,5-Difloro-2-nitroaniline with HF/6-311++G(d,p)

Table 4.1 Comparison of the experimental (FT-IR and FT-Raman) and computed vibrational frequencies of 4,5-Difloro-2-nitroaniline

Experimental		Calculated				IR Intensity	Raman Intensity	PED >10%
		HF		DFT				
IR	Raman	**Unscaled**	scaled	**Unscaled**	scaled			
3740(s)		3985	3745	3714	3639	58.56	58.19	$\nu_{as}NH_2[\nu N_9H_{10}(74) + \nu N_9H_{11}(26)]$
3628(vw)		3842	3611	3548	3477	77.28	151.64	$\nu_{s}NH_2[\nu N_9H_{10}(74) + \nu N_9H_{11}(26)]$
2356(vs)	3345(vw)	3423	3217	3245	3180	14.10	43.89	$\nu C_3H_7(99)$
		3386	3182	3211	3146	0.37	90.82	$\nu C_6H_8(99)$
1696(m)		1839	1728	1684	1650	191.82	7.97	$\nu [\nu C_3\text{-}C_4(10) + \nu C_6\text{-}C_5(12)+\nu C_2\text{-}C_3(15)+\beta H_{11}\text{-}N_9\text{-}H_{10}(18)$
1648(w)	1611(vw)	1833	1723	1664	1630	90.81	3.93	$\beta H_{11}\text{-}N_9\text{-}H_{10}(18)$
	1572(vw)	1756	1650	1608	1577	102.76	26.93	$\nu C_3\text{-}H_4(11)+ \nu C_5\text{-}C_4(29)+\beta C_6\text{-}C_5\text{-}C_4(10)+\beta C_1\text{-}C_6\text{-}C_5(14)$
	1509(m)	1689	1655	1550	1519	276.16	3.42	$\nu C_5\text{-}C_4(11)+ \nu N_9\text{-}C_1(12)+\beta H_7\text{-}C_3\text{-}C_2(13)+\beta H_8\text{-}C_6\text{-}C_1(17)$
1519(vw)	1441(w	164	1548	1508	1477	31.55	5.31	$\nu C_6\text{-}H_5(27)+ \nu N_9\text{-}$

	)	7						C_1(15)
1463(w)	1380(s)	1549	1456	1418	1389	68.71	39.59	νC_3-C_4(14) + νC_6H_5(12) +νN_9C_1(10)+ $\nu O_{13}N_{12}$(17)+ $\beta H_{10}N_9C_1$(12)
1395(w)	1335(m)	1492	1402	1401	1372	56.22	64.19	νC_3H_4(16) + $\nu O_{13}N_{12}$(30) + νC_1C_6(15)
1370(w)		1450	1363	1339	1312	82.62	13.28	νC_2C_3(45) + νN_9C_1(14)+ $\nu O_{14}N_{12}$(10)
	1276(s)	1399	1315	1286	1260	22.16	2.63	+β $H_7C_3C_2$(36) + β $H_8C_6C_1$(35)
	1245(s)	1361	1279	1253	1227	263.86	77.44	$\nu N_{12}C_2$(11)+ $\nu F_{15}C_4$(13)+ β $H_7C_3C_2$(16)
	1203(vs)	1344	1263	1236	1211	315.56	100.33	$\nu O_{13}N_{17}$(17)+ $\nu O_{14}N_{12}$(29)
		1279	1202	1180	1156	12.38	4.66	$\nu F_{16}C_5$(30)+ β $C_2C_3C_4$(15)+ β $C_6C_5C_4$(11)
	1086(m)	1188	1116	1092	1070	1.65	8.75	νC_1C_6(20)+ β $H_{10}N_9C_1$(47)
1052(w)	993(w)	1163	1093	1068	1046	20.09	2.15	$\nu N_{12}C_2$(16)+ $\nu F_{16}C_5$(10)
		1060	996	939	920	54.58	0.85	$\tau H_7C_3C_2N_{12}$(82)
	875(m)	933	877	852	834	45.31	4.93	$\nu F_{15}C_4$(17)
		933	877	838	821	25.32	0.89	$\tau H_8C_6C_1N_9$(73)
	790(s)	855	803	771	755	33.54	29.78	νC_5C_4(14)+ β $O_{14}N_{12}O_{13}$(40)
	721(vw)	811	762	754	738	0.05	11.18	νC_5C_4(22)+ $\nu F_{16}C_5$(11)+ $\nu F_{15}C_4$(13)+ $\beta C_5C_4C_3$(18)
		785	737	709	694	144.55	1.22	$\tau H_{11}N_9C_1C_6$(77)
		741	696	687	673	38.45	1.01	$\gamma O_{14}C_2O_{13}N_{12}$(62)
659(m)		728	684	649	636	18.84	0.39	$\nu F_{16}C_5$(10)+ $\beta C_1C_6C_5$(11)+ $\gamma O_{14}C_2O_{13}N_{12}$(12)
		705	662	648	635	18.21	2.5	$\beta F_{15}C_4C_5$(25)+ $\gamma N_9C_6C_2C_1$(37)
	611(w)	688	646	625	612	1.57	0.07	$\gamma F_{16}C_4C_6C_5$(30)+ $\gamma N_9C_6C_2C_1$(21)
		659	619	602	589	3.54	4.16	$\beta C_6C_5C_4$(19)+ β $N_9C_1C_2$(10)+ β $O_{13}N_{12}C_2$(11)

	496(w)	529	497	507	496	111.54	0.23	$\tau H_{10}N_9C_1C_6(89)$
		519	487	490	480	6.80	9.04	$\nu C_6C_5(13)+ \beta O_{13}N_{12}C_2(18)+ \beta C_1C_6C_5(21)$
		497	467	447	438	10.13	0.52	$\tau C_2C_3C_4C_5(50)$
		465	437	428	419	1.85	8.22	$\beta C_5C_4C_3(13)+ \beta O_{13}N_{12}C_2(37)$
		420	394	380	372	5.5	1.5	$\beta N_9C_1C_2(46)+ \gamma F_{16}C_4C_6C_5(18)+ \gamma F_{15}C_3C_5C_4(46)$
		405	380	378	370	2.08	0.22	
		391	367	365	357	0.05	8.88	$\nu N_{12}C_2(27)+ \beta C_2C_3C_4(18)+ \beta C_5C_4C_3(14)$
		300	282	274	268	1.01	0.41	$\beta F_{16}C_5C_6(44)+ \beta F_{15}C_4C_6C_5(35)$
		282	265	235	249	0.09	1.40	$\tau C_1C_6C_5C_4(41)+ \gamma F_{16}C_4C_6C_5(14)$
		256	240	238	233	5.13	0.65	$O_{13}N_{12}C_2(12)+ \beta N_{12}C_2C_3(53)+ \beta F_{15}C_4C_5(17)$
		185	173	169	165	0.22	0.84	$\tau C_1C_6C_5C_4(14)+ \tau F_{15}C_3C_5C_4(24)+ \tau N_{12}C_3C_1C_2(31)$
		109	102	102	99	3.75	0.06	$\tau C_6C_5C_4C_3(45)+ \tau C_1C_6H_5C_4(18)$
		62	58	72	70	0.01	0.53	$\tau O_{13}N_2C_2C_3(19)$

Unit in cm-1. Abbreviations: w- weak, vw-very weak, s- strong, m- medium vs- very strong ν – stretching, νas- asymmetric stretching, νs -symmetric stretching, τ-torsion, β –in plane bending, γ-out of plane bending.

5. CONCLUSION

In the present investigation of the molecule 4,5-difloro-2-nitroaniline a detailed geometrical, and vibrational analysis have been done with the help of both empirical quantum chemical method Hartree Fock and density functional theory. This is the first time that optimized structure, vibrational frequencies, produced for the title compound 4,5-difloro-2-nitroaniline. The data obtained from the above analysis with different basis sets by HF and DFT give good agreement with the experiment one. The scaled vibrational frequencies of all modes of title compound 4,5-difloro-2-nitroaniline are in expected range and almost equal to obtained from experimental data.In the light of this work, it is observed that there is an insignificant difference between the values reported by two theories but DFT has an advantage over HF.

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