Spectroscopic nvestigation (*FT-Raman , FTIR and SERS*), HOMO-LUMO and Mullikan Population Analysis Study of 1-Fluoro 4-Nitrobenzene

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Abstract—**In this study, the experimental and theoretical vibrational frequencies of a newly synthesized 1-Fluoro 4-Nitrobenzene are investigated. The experimental FTIR (250-4000cm-1)and Raman spectra (0-4000) cm-1 of the molecule in solid phase are recorded. A surface –enhanced Raman scattering(SERS) spectra in the region (400-5000cm-1).The theoretical vibrational frequencies and optimized geometric parameters (bond length and bond angles) are calculated by using Density Functional Theory (DFT/B3LYP: Becko, 3-parameter,(Lee-Yang-parr) and Quantum Chemical Methods (with 6-311**G basis set by Gaussian 09W software) for the first time . The assignment of the vibrational frequencies are done by Mulliken population analysis by using Gaussian 09W software. The theoretical optimized geometric parameters and vibrational frequencies are found to be in good agreement with the corresponding experimental data . In addition, the Highest Occupied Molecular Orbital (HOMO) and the Lowest Unoccupied Molecular Orbital(LUMO) are calculated at B3LYP/6-311**G level .**

Keywords-component; 1-Fluoro 4-Nitrobenzene: FT-Raman: FTIR: SERS: HOMO-LUMO.

I. INTRODUCTION

The Surface enhanced Raman Scatterig (SERS) has proved to be one of the most senstive spectroscopic techniques for chemical analysis. It is also used for single molecule detection[1]. This technique is used in chemistry, biology and physics of materials, and many other scientific areas, where vibrational spectroscopy is required. SERS can give extremely efficient information about the Vibrational structure of a molecule.

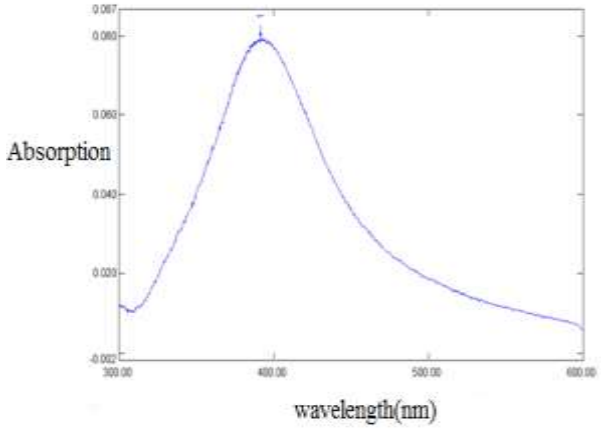
DFT calculations have recently become an efficient tool in the prediction of geomentry of molecular structure, Mulliken structure and vibrational wavenumbers (FTIR and Raman) these methods predict relatively accurate molecular structure and vibrational spectra with moderate computational effort. In particular for atomic molecule, the DFT methods lead to the prediction of more accurate molecular structure and also vibrational wavenumbers. From spectroscopic point of view the spectra of derivatives of nitrobenzene have been studied extensively. Therefore in the present work, the vibrational wavenumbers, mulliken population analysis, HOMO-LUMO energy gap were investigated by using B3LYPcalculation with 6-311**G basis sets.

II. EXPERIMENTAL DETAILS

A. Preparation of Silver sol using Creighton Method

Silver sol, for SERS studied, was prepared by Creighton method [2]. The UV Absorption spectrum of the silver sol, recorded using SHIMADZU UV- 1650 pc, UV- VIS recording spectrometer, shows a single absorption band at 391, as shown in Fig.1, confirming the formation of silver nanoparticles.

Figure 1. UV-Visible Absorption Spectrum of Silver Sol



B. Preparation of samples- 1-Fluoro 4-Nitrobenzene with Silver Sol

The compound under investigation, 1-Fluoro 4-Nitrobenzene, was purchased from Safire scientific Company, Coimbatore. The sample solutions was mixed with the Silver sol with sample-sol ratios 1:20, 1:10 and 1:5 thus preparing three sets of solutions as shown below.

A= 0.5 ml (Solution) with 2.5ml (Silver Sol)

B=0.5 ml (Solution) with 5ml (Silver Sol)

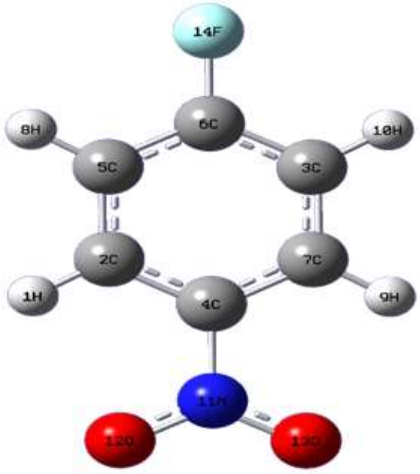
C=0.5 ml (Solution) with 10 ml (Silver sol)

The Raman spectra of the liquid sample, solutions at different concentrations, and solutions mixed with silver sol were recorded using 1064 nm Nd:YAG laser line as the excitation frequency using the Bruker RFS Raman spectrometer. These are shown in Fig.2 and Fig.3.

III. COMPUTATIONAL DETAILS

The Optimized geometry of 1-Fluoro 4-Nitrobenzene and vibrational frequencies were calculated by Gaussian 09W program package[3] with B3LYP/6-311**G method. The vibrational wave numbers were calculated using the Gaussian 09 software package on a personal computer. The computations were performed at B3LYP/6-311**G level of theory, to get the optimized geometry Fig.7. optimized fig and vibrational wavenumbers of the normal modes of the title compound values are given in Table.1. DFT calculations were carried out with Becke's three parameter hybrid model using the Lee-Yang-Parr correlation functional (B3LYP) method[4]. Molecular geometries were fully optimized by Berny's optimization algorithsm using redundant internal coordinates. Mulliken population analysis , HOMO-LUMO were carried carried out by using B3LYP/6-311**G level.

Figure 7. Optimized geometry of 1-Fluoro 4-Nitrobenzene



IV. GEOMENTRICAL PARAMETERS

The DFT calculations of the 1-Fluo 4-Nitrobenzene for the bondlength of C2-C1=1.3947Å and C3-C2=1.3954 Å respectively[5,6]. In the present case of the DFT calculations give C4-C3 bondlength as 1.3948 Å and H1-H6 bondlength as 1.0996 Å give the corresponding bondlength of H2-H1=1.0996 Å give the corresponding bondlength of H2-H1=1.0996 Å whereas in the present cese corresponding value is H4-H3 bondlength for 1.0996 and hydrogen atom H5-H4 bondlength as 1.0997 Å, F3-F2= 1.3499 and also bondlength as N6-N1=1.4699in Table.2 and also shown in Fig.8. respectively.

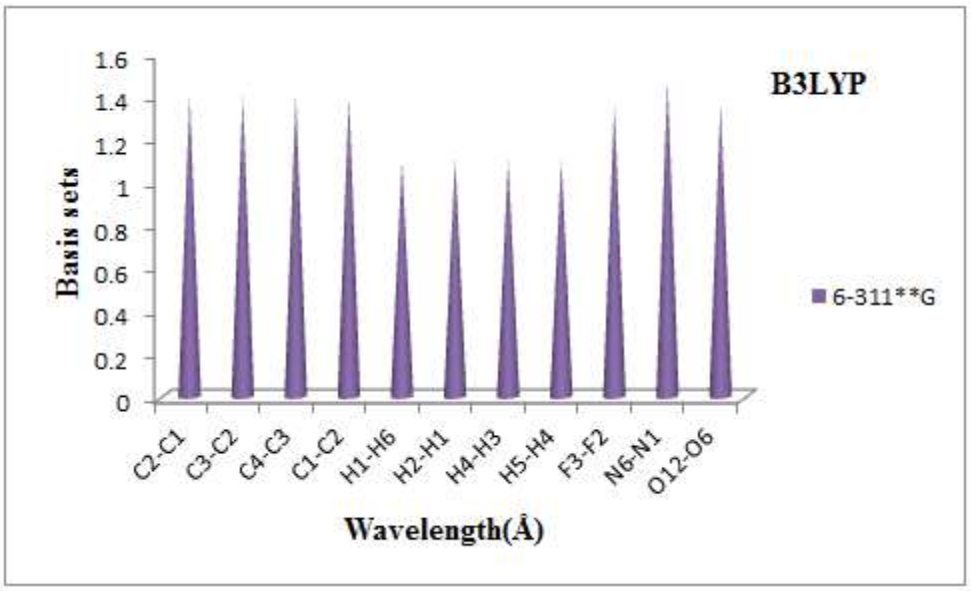
TABLE I. DFT OF THE 1-FLUORO 4-NITROBENZENE CALCULATED AT B3LYP/6-311**G LEVEL (BONDLENGTH(Å)),(BONDANGLES(˚)

1 -Fluoro 4-Nitrobenzene (B3LYP)	
Parameters	***6-311**G***
Bond length(Å)	
C2-C1	1.3947
C3-C2	1.3954
C4-C3	1.3948
C1-C2	1.3948
H1-H6	1.0996
H2-H1	1.0996
H4-H3	1.0996
H5-H4	1.0997
F3-F2	1.3499
N6-N1	1.4699
O12-O6	1.36

1-Fluoro 4-Nitrobenzene (B3LYP)	
Parameters	***6-311**G***
Bond Angles(˚)	
C3-C2-C1	119.9941
C4-C3-C2	119.994
C1-C2-C3	119.9934
H1-H6-H5	120.0043
H2-H1-H6	119.9807
H4-H3-H2	119.981
H5-H4-H3	120.0113
F3-F2-F1	120.0128
N6-N1-N2	120.0079
O12-O6-O1	109.4712

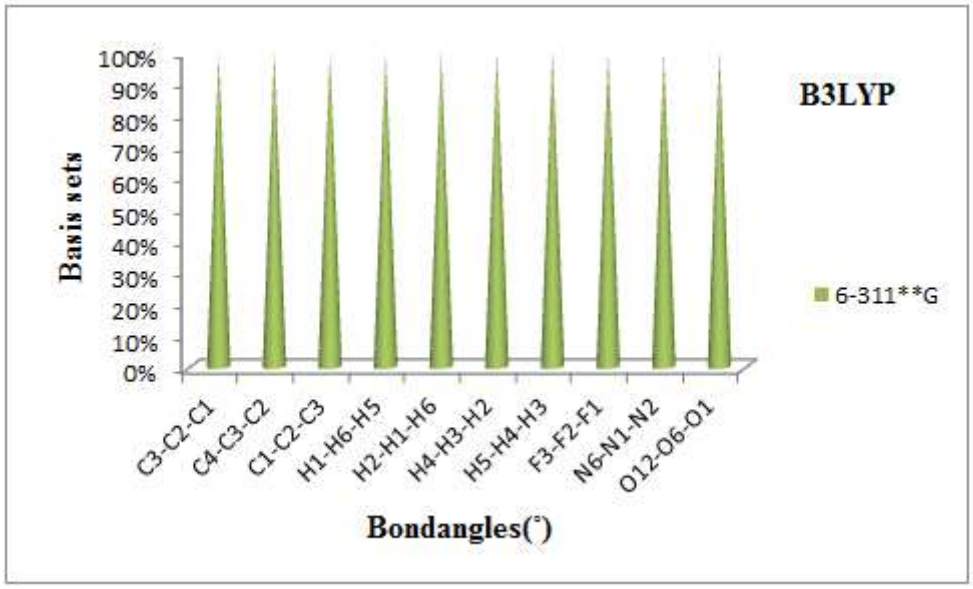
The expected bondangle for this compound(C1-C2-C3,C2-C3-C4) in 119 ˚. For the title compound the theoretically obtained values are given in Table.3.It can be seen that it is slightly different from near expected value. This is due to the fact that the theoretically calculated value is gaeous face (single molecule).

Figure 8. DFT of the 1-Fluoro 4-Nitrobenzene calculated at B3LYP/6-311**G level (bondlength(Å))



DFT calculations give the bond-angle is C1-C2-C3 bond angle is 119.9934˚ and also the bond angle of H2-H1-H6=119.9801˚, H1-H6-H5=120.0043˚, H4-H3-H2=119.9810˚, H5-H4-H3=120.0113˚. similar to the measured value in hydrogen [7,8]. The F3-F2-F1 of bond angle is 120.0128˚ and also the O12-O6-O1=109.4717˚ slightly longer than N6-N1-N2=120.0079˚ bond of the ring shown in Table.2. and also shown in Fig.9.respectively.

Figure 9. DFT of the 1-Fluoro 4-Nitrobenzene calculated at B3LYP/6-311**G level (bondangles(˚))



V. PREDICTION OF RAMAN INTENSITIES

The Raman activities (Si) calculated by Gaussian 09 program [9] converted to relative Raman intensities(Ii) using the following relationship derived from the intensity theory of Raman scattering[10,11]

$$I_i = \frac{f(v_o - v_i)^4 S_i}{v_i[1 - \exp(-hcv_i/kt)]} \quad (1)$$

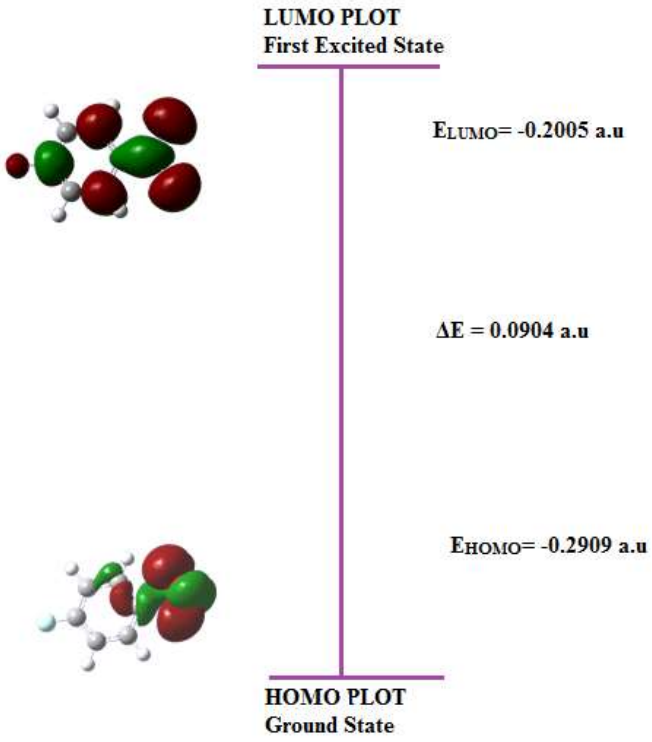
Where υo is the exciting wave numbers in cm-1,υi the vibrational wavenumbers of the ith normal mode. h,c and k are fundamental constants and f is a suitablychosen common normalization factor for all peak intensities. For simulation the calculated FT-Raman spectra has been plotted using pure Lorentzian band shape with a bandwidth (FWHM) of 10cm-1 as shown in Fig.2 and Fig.3(Theoretical) along with Theoretical FTIR spectra.

VI. HOMO-LUMO ANALYSIS

Many organic molecules containing conjugated π electrons have been characterized as hyper polarizabilities and researched by means of vibrational spectroscopy the π electron cloud moment from donor to acceptor can make the molecule highly polarized through the single-double path when it changes from the ground state to the excited state. Both the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) are the main orbitals talking part in chemistry stability, the HOMO represents the ability to donate an electron, LUMO as an electron acceptor represents the ability to obtain an electron [12]. The HOMO and LUMO energies have been calculated by B3LYP/6-311**G methods and depicted Fig.10. considering chemical hardness, large HOMO-LUMO gap means a soft molecule one can also related the stability of the molecule to hardness. which means that molecule with least HOMO-LUMO gap means it is more reactive[13]. The frontier molecules orbital, HOMO and LUMO and frontier orbital energy gap helping to amplify the reactivity and kinetic stability of molecules are important parameters in the electronic studies[14,15] the analysis of the wave function indicates that the electron absorption corresponding to the transition from the ground state to the first excited state is

mainly defined by one electron excitation from the highest occupied molecular orbital (HOMO) to the lowest unoccupied molecular orbital(LUMO)[16].the HOMO-LUMO energy gap calculated at B3LYP/6-311**G level reflect the chemical activity of the molecule and explain the eventual charge transfer interaction with in the molecule which influences the biological activity of the molecule. The positive phase is represented in red colour and negative phase is represented in green colour. The HOMO LUMO plots are shown in Fig.10.

Figure 10. Calculated HOMO-LUMO Plots of 1-Fluoro 4 –Nitrobenzene and HOMO-LUMO gap



VII. MULLIKEN POPULATION ANALYSIS

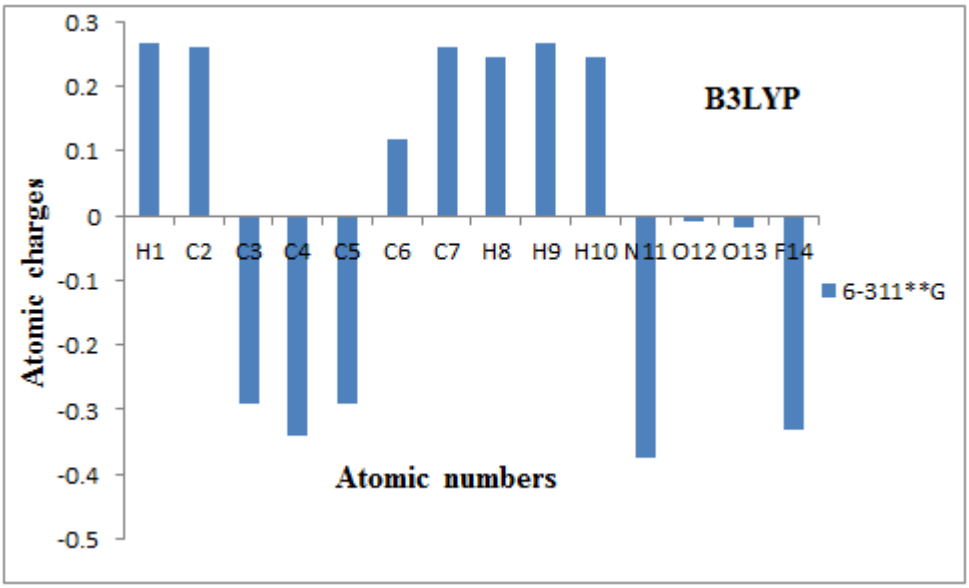
The bonding capability of molecules depends on the electronic charge on the chelating atoms and hence the atomic charge values were obtained by the Mullikan population analysis [17]. To validate the reliability of the results, the Mullikan population analysis of 1-Fluoro 4-Nitrobenzene molecules are calculated using B3LYP/6-311**G method and basis sets. The corresponding characteristics of the atomic charge population of the constituent atoms are presented in Table.4. for 1-Fluoro 4-Nitrobenzene respectively.

TABLE IV. MULLIKEN ATOMIC CHARGES OF 1-FLUORO 4-NITROBENZENE PERFORMED BY B3LYP/6-311**G METHODS.

Atoms	**Mulliken Atomic charge**
	B3LYP/6-311**G
H1	0.266
C2	0.261
C3	-0.29
C4	-0.34
C5	-0.29
C6	0.117
C7	0.261

H8	0.245
H9	0.266
H10	0.245
N11	-0.374
O12	-0.01
O13	-0.018
F14	-0.332

Figure 11. The Mulliken plot structure of 1-Fluoro 4-Nitrobenzene



In 1-Fluoro 4-Nitrobenzene, the negative values on C3, C4, C5, N11, O12, O13 and F14 atoms of Fluoro group in the aromatic ring leads to a redistribution of electron density due to these strong negative charge. H1 and H9 higher positive charged they become bonded to the hydrogen atom and all oxygen atoms are electron acceptor and also indicates the charge transfer from oxygen to hydrogen. The mulliken plot structure of 1-Fluoro 4-Nitrobenzene are shown in Fig.11 respectively.

VIII. RESULT AND DISCUSSION

A. FT-IR and Raman Spectrum

The FT-IR and FT-Raman Spectrum of 1-Fluoro 4-Nitrobenzene Shown in Fig.2 and Fig.3 respectively. The wavenumbers of the observed FTIR and Raman bands calculated values using B3LYP/6-311**G levels and the assignments are given in table.4.

B. C-H vibrations

In aromatic compounds, the C-H stretching frequencies appear in the range 3100-3000cm-1 [18]. C-H in plane bending mode appears in the range of 1300-950cm-1 and the C-H out of plane bending vibrations appear in the region 950-670cm-1[19]. Hence the FTIR bands observed at 3094, 3128, 3146, 3226, 3230 cm-1 in 1-Fluoro 4-Nitrobenzene respectively. And the Raman bands observed at 3226cm-1.The C-H in plane bending vibrations of 1-Fluoro 4-Nitrobenzene FTIR bands observed at 1527cm-1. The symmetric bending vibration have been also identified for 1-Fluoro 4-Nitrobenzene FTIR bands observed at 1519cm-1 were presented in Table.1 respectively.

C. C-C vibration

The ring carbon- carbon stretching vibration occurs in the region 1650-1400cm-1 [20] therefore, the C-C stretching vibration of 1-Fluoro 4-Nitrobenzene are found at FTIR bands observed at 1466,1469,1495,1595,1622,1629cm-1 and the Raman bands observed at 1480,1595,1616,1622 cm-1 of the title compound. The 1-Fluoro 4-Nitrobenzene were well identified in the recorded spectra within their characteristic region and also listed in Table.1. The C-C out of plane bending of FTIR bands observed at 503cm-1.

Figure 2. Comparison of observed and calculated FTIR spectra of the title compound

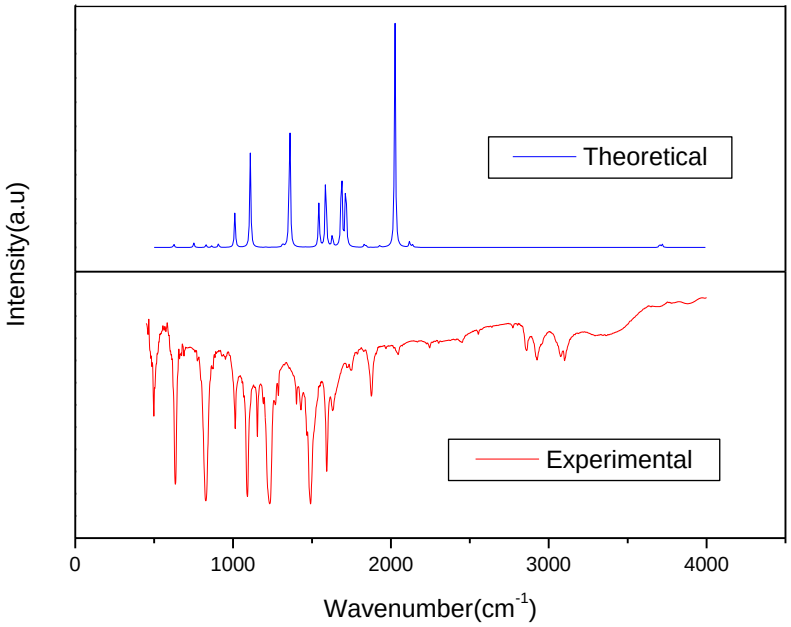


Figure 3. Comparison of observed and calculated Raman spectra of the title compound

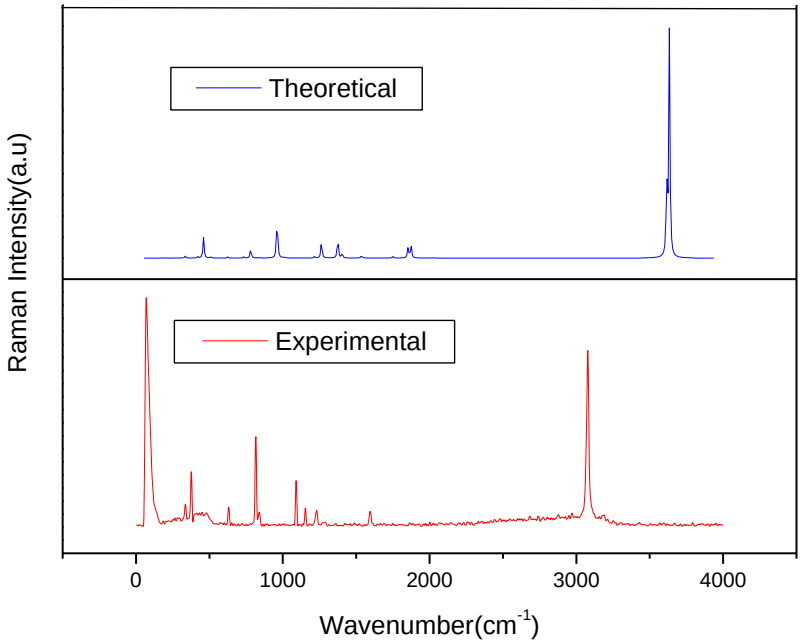


TABLE 1. THE OBSERVED AND EXPERIMENTAL (FTIR, FT-RAMAN) ASSIGNMENTS OF 1-FLUORO 4-NITROBENZENE USING B3LYP/6-31+G* CALCULATIONS.

B3LYP/6-311G**		**Observed Frequency(cm-1)**		**SERS(cm-1)**			**Assignments (%)**
Calculated Frequency(cm-1)							
FTIR	***Raman***	***FTIR***	***Raman***	***A***	***B***	***C***	
486	-	487	-	-	-	-	t R asymd
-	-	-	-	-	499	499	ωCC
-	-	503	-	-	-	-	ωCC
-	-	529	-	-	-	-	υCC
616	-	-	-	-	-	-	t R asymd
-	-	621	-	-	-	-	t R asymd
-	-	-	635	635	635	635	t R asymd
-	-	681	-	-	-	-	bCO
-	-	741	747	747	-	-	R assymd
-	-	757	-	-	803	-	R assymd
-	-	809	-	-	-	-	υCH
-	-	-	814	814	-	-	υCH
842	-	-	-	848	848	848	υCH
851	-	-	859	-	-	-	$^{\delta}$NO2
868	-	867	-	-	-	-	$^{\delta}$CH3
894	-	-	-	-	-	-	ωCH
-	-	995	-	-	-	-	$^{\delta}$Ph(I)
-	-	1011	-	-	-	-	υCN
1050	-	-	-	-	-	-	υCF
-	-	1087	-	-	-	-	υPh(I)
-	-	-	-	-	-	1096	υCC
-	-	-	-	1109	1109	-	υCC
-	-	1113	-	-	-	-	υCC
	1128	1121	1120	-	1120	-	bCH
1137	-	-	-	-		1131	CH3opr
-	-	1141	-	1141	-	-	CH3opr
-	-	-	-	-	1155	1155	bC=O
1188	-	-	-	-	-	-	bCH
	1197	-	-	-	-	-	bCH
-	-	1215	-	-	-	-	bCH
-	-	-	-	1243	-	1243	bCH
--	-	1257	1256	-	1256	-	bCH
1284	1284	-	-	-	-	-	bCH
-	-	1291	-	-	-	-	$^{\delta}$CH
-	-	-	-	1347	1347	1347	bOH
-	-	1351	1357	-	-	-	bOH
1362	-	-	-	-	-	-	bOH
1431	-	-	-	-	-	-	bCH

1466	-	1469	-	-	-	-	υCC
-	-	-	1480	-	-	-	υCC
-	-	1495	-	1493	-	1493	υCC
-	-	1519	-	1515	-	-	CH3sb
1527	-	-	-	-	-	-	CH3ipb
-	-	-	1539	-	1539	1539	bCH
-	-	-	1539	-	1539	1539	bCH
-	-	-	-	1584	-	-	υCC
-	-	1595	1595	-	1595	-	υCC
-	-	-	-	1605	-	1605	υCC
-	-	-	1616	-	-	-	υCC
1622	1622	1629	-	-	-	-	υCC
-	-	-	1741	-	-	-	υC=O
-	-	1773	-	-	-	-	υC=O
-	-	1825	-	-	-	-	υC=O
-	-	1875	-	-	-	-	υC=O
-	-	1917	-	-	-	-	υC=O
-	-	1951	-	-	-	-	υC=O
-	-	2045	-	-	-	-	υC=O
-	-	2105	-	-	-	-	υC=O
-	-	2223	-	-	-	-	υC=O
-	-	2256	-	-	-	-	υC=O
-	-	2392	-	-	-	-	υC=O
-	-	-	2453	-	-	-	υC=O
-	-	2460	-	2464	2464	2464	υC=O
-	-	2612	-	-	-	-	υC=O
-	-	-	2645	-	-	-	υC=O
-	-	2654	-	-	-	-	υC=O
-	-	-	-	2677	-	-	υC=O
-	-	2696	-	-	2690	-	υC=O
-	-	2782	-	-	-	-	υSCH2
-	-	2866	-	-	-	-	υSCH2
-	-	2942	-	-	-	-	υasCH2
-	-	2992	-	-	-	-	υsCH2
-	-	3094	-	3095	3095	3095	υCH
-	-	3128	-	-	-	-	υCH
-	-	3146	-	-	-	-	υCH
-	-	-	-	-	3175	-	υCH
-	3200	3230	-	-	-	-	υCH
3226	3226	-	-	-	-	-	υCH
-	-	3450	-	-	-	-	υOH

Abbreviations: ω= out of plane bending, asymd= antisymmetric deformation, opr= out of plane rocking , υ= stretching, sb=symmetric bending, ipb=in plane bending ,b=bending ,b= bending, trigd= trigonal deformation , ph(I)= tri and para substituted phenyl rings, sb= symmetric bending,$^{\delta}$= in plane bending

A. O-H vibrations

The O-H group gives rise to three vibrations (stretching, in-plane bending vibration). The O-H group vibrations are likely to be most sensitive to the environment. So they show pronounced shifts in the spectra of the hydrogen bonded species. The hydroxyl stretching vibrations are generally [4] observed in the region around 3500cm-1. The O-H vibrations FTIR bands observed at 3450cm-1

B. υC=O vibration

The vibration belonging to the band between the ring and the halogen atom are important to discuss here, since mixing of vibration are possible due to lowering of the molecular geometry and the presence of heavy atom on the periphery of molecule [21] .The assignments of υC=O in the region 1500cm-1-2700cm-1. The υC=O in the FTIR bands observed at 1773, 1825, 1875, 1917, 1951, 2045, 2105, 2223, 2256, 2392, 2460, 2612, 2654, 2696 cm-1 and Raman bands observed at 2453, 2645 cm-1

In this study CH bending vibrations the Raman bands are observed at 1128, 1120, 1197, 1256, 1284, 1539 cm-1 similarly the FTIR bands observed at 1284, 1257, 1121, 1188, 1215, 1431 cm-1.The bending CO vibrations the FTIR bands observed at 681cm-1. The antisymmetric deformation of the FTIR bands observed at 486, 487, 621cm-1 and the Raman bands observed at 635cm-1 similarly asymmetric of the FTIR bands observed at 741, 757cm-1 and Raman bands observed at 747cm-1

C. υCC vibrations

υCC vibrations Raman bands observed at 1480cm-1 and FTIR bands observed at 529, 1113, 1466, 1469, 1495cm-1. In the vibrational spectra of related compounds the bands due to bending vibration the FTIR bands observed at 1351, 1362 cm-1 and the Raman bands observed at 1357cm-1. In the present investigation, the FTIR bands observed at 842, 809cm-1 and Raman bands observed at 814cm-1 is assigned to CH-stretching vibrations for 1-Fluoro 4-Nitrobenzene.

D. υCF vibrations

The most characteristics features of NO2 in plane bending the FTIR bands observed at 851cm-1 similarly the Raman band observed at 859cm-1. CH3 in plane bending of FTIR bands observed at 868, 867cm-1 .Generally, the CH out of plane bending modes of the FTIR bands observed at 894cm-1. The in plane bending of tri and para substituted phenyl rings bands of FTIR spectrum observed at 995 cm-1 similarly stretching tri and para substituted phenyl rings bands of FTIR spectrum at 1087cm-1. In the present investigation of the CN stretching vibrations FTIR bands observed at 1011cm-1 similarly the CF stretching vibrations FTIR bands observed at 1051cm-1.

E. CH3 rocking

The vibration belonging to the band between the ring and the hydrogen atom are important to disscuss here, since mixing of vibration are possible of the molecular symmetry and the presence of heavey atom on the periphery of molecule [21] the assignments of CH3 out of plane rocking of the FTIR band observed at 1137, 1141cm-1. The CH in plane bending of FTIR bands observed at 1291cm-1. The υs CH2 vibrations of the FTIR bands observed at 2782, 2866, 2992cm-1 similarly the υas CH2 vibrations of the FTIR spectrum at 2942cm-1. The stretching OH vibrations of FTIR bands observed at 3450cm-1.

IX. SERS SPECTRAL ANALYSIS

The SERS spectrum analysis of 1-Fluoro 4-Nitrobenzene Fig 4,5,6, has been recorded and the vibrational analysis is performed by comparing its with the normal Raman spectrum. The vibrational modes, the observed wavenumbers measured SERS and Raman bands positions and their tentative assignments are given in Table.1.

Figure 4. Raman and SERS spectra of 1-Fluoro 4-Nitrobenzene (0 to 1000 cm-1)

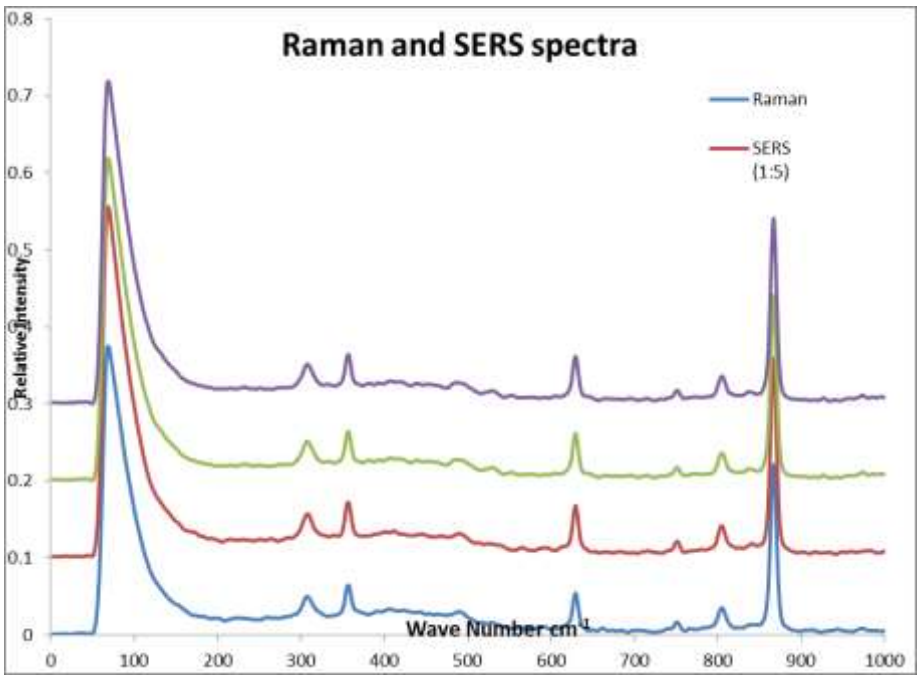


Figure 5. Raman and SERS spectrum of 1-Fluoro 4-Nitrobenzene (1000-1450cm-1)

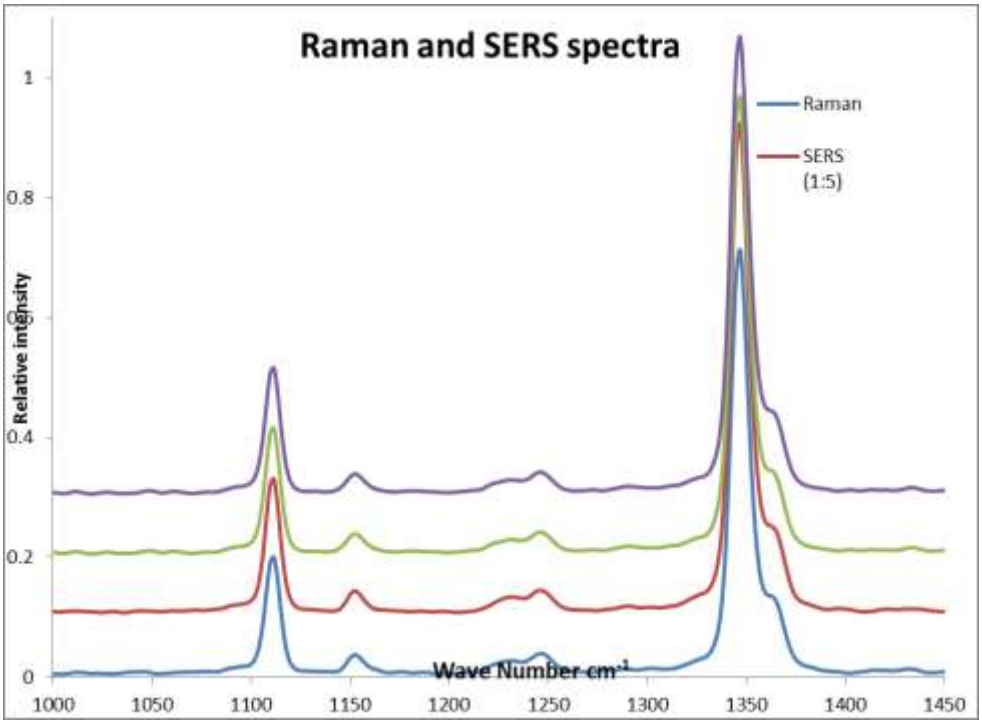
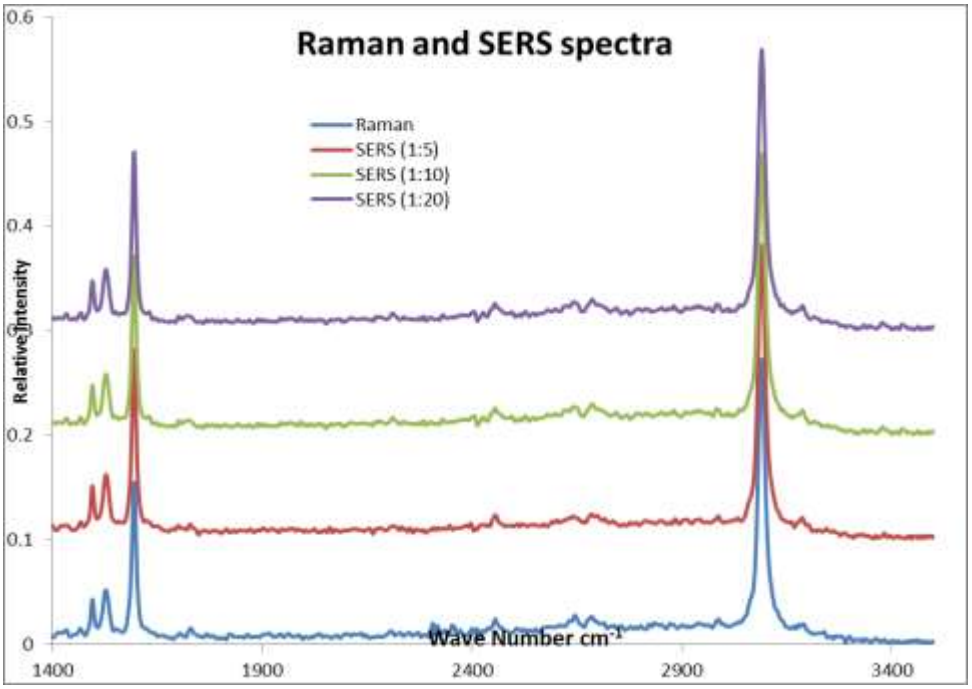


Figure 6. Raman and SERS spectra of 1-Fluoro 4-Nitrobenzee (1400 to 3400 cm-1)



The adsorption mechanism of an adsorbate can be deduced from its SERS spectrum. The possible potential sites available for the adsorption of 1-Fluoro 4-Nitrobenzene on a surface as a benzene ring The system and the fluoro group. The orientation of the molecule on the surface can be inferred from aromatic C-H stretching vibrations, CH bending, OH bending vibrations and the SERS surface selection rule [22,23]. In the SERS spectrum of 1-Fluoro 4-Nitrobenzene Fig.4,5,6, CH stretching to SERS band observed at 814,848cm-1 both bands are very strong, indicating that the interaction between the benzene ring of 1-Fluoro 4-Nitrobenzene molecules of good enhancement. The CC stretching vibrations of SERS band observed at 1096, 1109, 1493, 1584, 1595, 1605cm-1 are good enhancement in the SERS spectrum. The relativity strong enhancement of the 3175, 3095cm-1 band assigned to the CH stretching vibrations, indicate that the adsorption of 1-Fluoro 4-Nitrobenzene takes place through CH vibrations. In the SERS spectrum a strong bands at 2464, 2677, 2690 cm-1 that contain contribution of the C=O stretching vibrations. It is also informative to observe that the CH bending bands at 1539, 1120, 1243, 1256cm-1 with respect to the OH bending band at 1347cm-1 much more intense [22,23]. In a title geometry, the relative intensity of CH3 symmetric bending vibrations of the SERS band observed at 1515cm-1. According to the surface selection rules for Raman scattering [24-30]. It has been well-established that presence of the C=O bending vibration of the SERS bands observed at 1155cm-1 respectively. Hence the presence of the CH3 out of plane rocking of SERS band observed at 1131, 1141cm-1. The CC out of plane bending vibrations appear in the SERS bands observed at 499cm-1. The assymetric deformation of SERS band observed at 747, 803 cm-1 similarly the t R assymd SERS band observed at 635cm-1.

X. CONCLUSION

In this work the structure of molecule 1-Fluoro 4-Nitrobenzene have been obtained at the RB3LYP/6-31+G* level of theory. The title molecule was found to in the same plane modeling performed for 1-Fluoro 4-Nitrobenzene at the B3LYP/6-311**G level allowed the assignments of the FTIR and Raman bands of the compound, and was accurate vibrational frequencies and the vibrational spectra were well resolved. the experimental theoretical structural and vibrational investigations of 1-Fluoro 4-Nitrobenzenewere successfully confirmed by FTIR, Raman and differences observed between the experimental and computed values are carried out. The molecular structural, vibrational frequencies of the fundamental modes of the optimized geometry of 1-Fluoro 4-Nitrobenzene have been obtained from DFT calculation with 6-311**G levels. The theoretical results were compared with the experimental vibrations the substituent effect on the vibrational frequencies is analyzed. Both types of calculations have carefully explained the vibrational spectra of 1-Fluoro 4-Nitrobenzene. In this study through the difference between the calculated and experimental frequencies is very good agreement level of calculation. The calculated HOMO and LUMO energy show that the energy gap with in the molecule and also calculated mulliken population analysis are carried out.

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