

FT-Raman and FTIR Spectroscopic Investigation, First Hyper Polarizability, Homo-Lumo Analysis of P-Fluorobenzonitrile (PFBN)

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Abstract: *Quantum chemical density functional calculations were carried out for P-fluorobenzonitrile (PFBN) with the GAUSSIAN 09W using ab initio and Becke-3-Lee-Yang-Parr (B3LYP) functional. The observed FT-IR and FT-Raman vibrational frequencies are analysed and compared with theoretically predicted vibrational frequencies. The geometries and normal modes of vibration obtained from DFT method are in good agreement with the experimental data. The first-order hyperpolarizability (β) of the investigated molecule was computed using DFT calculations. The calculated HOMO and LUMO energies shows that charge transfer occur within molecule. The influences of nitrogen on the geometry of benzene and its normal modes of vibrations have also been discussed.*

Keywords: Ab initio, Vibrational Spectra, HOMO-LUMO, Hyperpolarizability

1. Introduction

Benzonitrile derivatives have a very interesting character in that three different binding sites (aromatic ring, π -bond of C-N group, and lone pair electrons of nitrogen atom) are available for the absorption of the molecule on the metal surface. Further, they are used as a solvent and chemical intermediate for the synthesis of pharmaceuticals, dyestuffs and rubber chemicals through the reactions of alkylation, condensation, esterification, hydrolysis, halogenation or nitration [93]. In addition to that they are used in the manufacture of lacquers, polymers and anhydrous metallic salts as well as intermediates for agrochemicals, and other organic chemicals. The vibrational spectral studies of the molecules can provide deeper knowledge about the relationships between molecular architecture, non linear response and hyperpolarizability. The infrared and Raman spectra in conjunction with quantum chemical computations, lead to precise information about the structure of the molecule.

For proper understanding of IR and Raman spectra, several theoretical methods, ranging from semi empirical to DFT approaches, are invaluable tools [2,3], each method having its own advantages. The Hartree-Fock (HF) level *ab initio* calculations have been performed to analyze the structural and vibrational characteristics of molecules. However, the use of post-HF level calculations, which include electronic correlation to the calculations, is necessary to get more reliable results on the structural parameters and vibrational properties. The density functional theory [4] has been accepted as a popular post-Hartree-Fock (HF) approach for the computation of molecular structure, vibrational frequencies and energies of molecule by the *ab initio* quantum chemistry community [5]. These *ab initio* and DFT computations have recently become an efficient tool in the prediction of molecular structure, harmonic force fields, vibrational frequencies, IR and Raman activities of

biological compounds [6]. The main focus of the present investigation is the study of the molecular structure and vibrational spectra of PFBN completely at HF and DFT levels using 6-311++G(d,p) basis set and to identify the various normal modes with greater wave number accuracy.

2. Experimental Details

The pure sample of PFBN was obtained from the Lancaster Chemical Company, UK and used as such for the spectral measurements. The room temperature Fourier transform infrared spectra of the title compound was measured in the region 4000-400 cm^{-1} at a resolution of $\pm 1 \text{ cm}^{-1}$ using a BRUKER IFS-66V FTIR spectrometer equipped with an MCT detector, a KBr beam splitter and globar source. Boxcar apodization was used for the 250 averaged interferograms collected for the sample and background.

The FT-Raman spectra of PFBN was recorded on a BRUKER IFS-66V model interferometer equipped with an FRA-106 FT-Raman accessory in the 3500 - 50 cm^{-1} Stokes region using the 1064 nm line of a Nd: YAG laser for excitation operating at 200mw power. The reported wave numbers are believed to be accurate within $\pm 1 \text{ cm}^{-1}$.

3. Computational Details

Quantum chemical density functional calculations were carried out for PFBN with the 2009 Window version of the GAUSSIAN suite program [7] using *ab initio* and Becke-3-Lee-Yang-Parr (B3LYP) functionals [8] supplemented with the standard 6-311++G(d,p) basis set (referred to as DFT calculations). All the parameters were allowed to relax and all the calculations converged to an optimized geometry which corresponds to a true energy minimum, as revealed by the lack of imaginary values in the wave number calculations.

The Cartesian representation of the theoretical force constants have been computed at the fully optimized geometry by assuming the molecule belongs to C_s point group symmetry. The transformation of force field from Cartesian to internal local-symmetry coordinates, the scaling, the subsequent normal coordinate analysis calculation of total energy distribution (TED), were done on a PC with the version V7.0-G77 of the MOLVIB program written by Sundius [9-11]. To achieve a close agreement between the observed and calculated frequencies, least-square fit refinement algorithm was used.

4. Results and Discussion

4.1 Molecular geometry

The molecular structure of P-fluorobenzonitrile is shown in Fig 1. The molecule under consideration would belong to C_s point group symmetry. The molecule has 13 atoms and one can expect 33 normal vibrations which are distributed as 23 in-plane vibrations (A' species) and 10 out-of-plane vibrations (A'' species). All the vibrations are active in both FTIR and Raman spectra. The global minimum energy obtained by the *ab initio* and DFT structure optimization for PFBN is calculated as -421.23172469 and -423.73708581

Hartrees, respectively. The calculated optimized geometrical parameters obtained in this study are presented in Table 1.

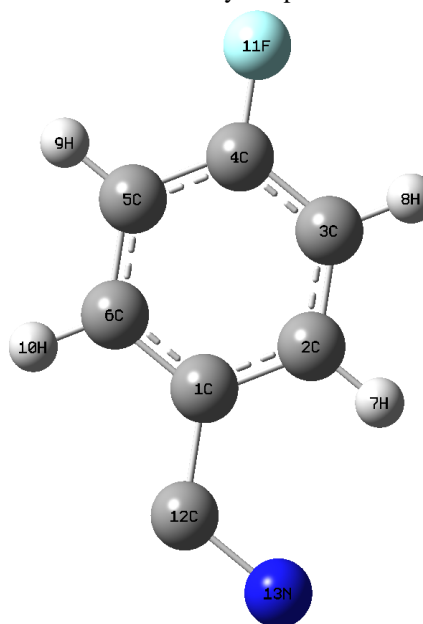


Figure 1: Optimized structure of PFBN PFM

Table 1: Optimized geometrical structural parameters calculated for Fluorobenzonitrile employing HF/6-11++G(d,p) and B3LYP/ 6-311++G (d,p) methods

Bond length	Value (Å)		Bond angle	Value (Å)		Dihedral Angle	Value (Å)	
	HF	B3LYP		HF	B3LYP		HF	B3LYP
C ₁ - C ₂	1.393	1.408	C ₂ - C ₁ - C ₆	120.0	119.8	C ₆ - C ₁ - C ₂ - C ₃	0.0	0.0
C ₁ - C ₆	1.393	1.408	C ₂ - C ₁ - C ₁₂	119.9	120.0	C ₆ - C ₁ - C ₂ - H ₇	180.0	180.0
C ₁ - C ₁₂	1.434	1.431	C ₆ - C ₁ - C ₁₂	119.9	120.0	C ₁₂ - C ₁ - C ₂ - C ₃	180.0	180.0
C ₂ - C ₃	1.384	1.393	C ₁ - C ₂ - C ₃	120.1	120.2	C ₁₂ - C ₁ - C ₂ - H ₇	0.0	0.0
C ₂ - H ₇	1.069	1.080	C ₁ - C ₂ - H ₇	119.8	119.7	C ₂ - C ₁ - C ₆ - C ₅	0.0	0.0
C ₃ - C ₄	1.376	1.387	C ₃ - C ₂ - H ₇	120.0	120.0	C ₂ - C ₁ - C ₆ - H ₁₀	180.0	180.0
C ₃ - H ₈	1.068	1.079	C ₂ - C ₃ - C ₄	118.2	118.2	C ₁₂ - C ₁ - C ₆ - C ₅	180.0	180.0
C ₄ - C ₅	1.376	1.387	C ₂ - C ₃ - H ₈	121.6	121.6	C ₁₂ - C ₁ - C ₆ - H ₁₀	0.0	0.0
C ₄ - F ₁₁	1.369	1.401	C ₄ - C ₃ - H ₈	120.0	120.1	C ₂ - C ₁ - C ₁₂ - N ₁₃	0.0	0.0
C ₅ - C ₆	1.384	1.393	C ₃ - C ₄ - C ₅	123.2	123.3	C ₆ - C ₁ - C ₁₂ - N ₁₃	180.0	180.0
C ₅ - H ₉	1.068	1.079	C ₃ - C ₄ - F ₁₁	118.3	118.3	C ₁ - C ₂ - C ₃ - C ₄	0.0	0.0
C ₆ - H ₁₀	1.069	1.080	C ₅ - C ₄ - F ₁₁	118.3	118.3	C ₁ - C ₂ - C ₃ - H ₈	180.0	180.0
C ₁₂ - N ₁₃	1.142	1.167	C ₄ - C ₅ - C ₆	118.2	118.2	H ₇ - C ₂ - C ₃ - C ₄	180.0	180.0

4.2 Vibrational Spectra

The vibrational analysis of PFBN are made the basis of the magnitude and relative intensity of the recorded spectra and in analogy with the assignment made by the earlier researchers on the similar type of molecules. The FTIR and

FT-Raman spectra of PFBN is shown in Fig.2 and 3, respectively. The detailed vibrational assignments of fundamental modes of PFBN along with the observed and calculated IR, Raman intensities, Reduced mass, Force constants and normal mode descriptions (characterized by TED) are reported in Table 4.

Table 2: Definition of Internal Coordinates of P-fluorobenzonitrile

No (i)	Symbol	Type	Definition ^a
Stretching			
1 - 4	P _i	CH	C3-H8, C2-H7, C5-H9, C6-H10
5	S _i	CF	C4-F11
6	R _i	CN	C12-N13
7 - 13	Q _i	CC	C1-C2, C2-C3, C3-C4, C4-C5, C5-C6, C6-C1, C12-C1
In-plane bending			
14 - 21	ψ _i	Ring	C1-C2-C3, C2-C3-C4, C3-C4-C5, C4-C5-C6, C5-C6-C1, C6-C2-C1, C6-C1-C7, C2-C1-C12
22 - 29	α _i	CCH	C1-C6-H10, C5-C6-H10, C6-C5-H9, C4-C5-H9, C1-C2-H7, C2-C3-H7, C2-C3-H8, C4-C3-H8
30 - 31	β _i	CC	C2-C1-C12, C6-C1-C12
32 - 33	σ _i	CF	C3-C4-F11, C5-C4-F11
34 - 35	φ _i	CN	(C6-C1)-C12-N13, (C2-C1)-C12-N13

Out-of-plane bending			
36 – 38	δ_i	CH	H10-C1-C6-C5, H9-C5-C4-C6, H8-C3-C2-C4
39	ϕ_i	CN	N13-C12-C1-(C2-C6)
40	ρ_i	CF	F11-C5-C3-C4
Torsion			
41 – 46	τ_i	tRing	C1-C2-C3-C4, C2-C3-C4-C5, C3-C4-C5-C6, C4-C5-C6-C1, C5-C6-C1-C2, C6-C1-C2-C3.

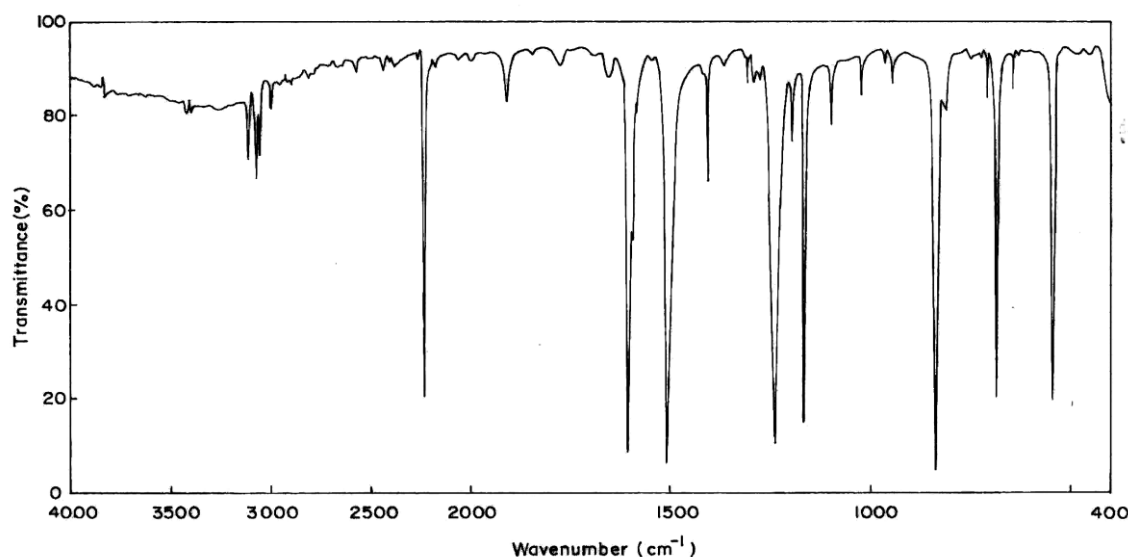


Figure 2: FTIR spectrum of P-fluorobenzonitrile

Detailed description of vibrational modes can be given by means of normal coordinate analysis (NCA). For this purpose, the full set of 46 standard internal coordinates (Containing 13 redundancies) were defined in Table 2. From these, a non-redundant set of local symmetry coordinates were constructed by suitable linear combination of internal coordinates following the recommendations of Fogarasi and Pulay [12,13] are summarized in Table 3. The theoretically calculated DFT force fields were transformed to this latter set of vibrational coordinates and used in all the subsequent calculations.

Table 3: Definition of Local Symmetry Coordinates of P-fluorobenzonitrile

No (i)	Symbol ^a	Definition ^b
1-4	CH	P_1, P_2, P_3, P_4
5-11	CC	$Q_5, Q_6, Q_7, Q_8, Q_9, Q_{10}, Q_{11}$
12	CF	S_{12}
13	CN	R_{13}
14-17	bCH	$(\alpha_{14}-\alpha_{15})/\sqrt{2}, (\alpha_{16}-\alpha_{17})/\sqrt{2}, (\alpha_{18}-\alpha_{19})/\sqrt{2}, (\alpha_{20}-\alpha_{21})/\sqrt{2}$
18	bCC	$(\beta_{22} - \beta_{23})/\sqrt{2}$
19	bCN	$(\beta_{24} - \beta_{25})/\sqrt{2}$
20	bCF	$(\beta_{26} - \beta_{27})/\sqrt{2}$
21	R trigd	$(\psi_{28} - \psi_{29} + \psi_{30} - \psi_{31} + \psi_{32} - \psi_{33})/\sqrt{6}$
22	R symd	$(-\psi_{28} - \psi_{29} + 2\psi_{30} - \psi_{31} - \psi_{32})/\sqrt{2}$

23	R asymd	$(\psi_{28} - \psi_{29} + \psi_{31} - \psi_{32})/\sqrt{12}$
24–28	ω CH	$\delta_{34}, \delta_{35}, \delta_{36}, \delta_{37}$
29	ω CN	ϕ_{38}
30	ω CC	Φ_{39}
31	ω CF	ρ_{40}
32	t R trigd	$(\tau_{41} - \tau_{42} + \tau_{43} - \tau_{44} + \tau_{45} - \tau_{46})/\sqrt{6}$
32	t R sym	$(\tau_{37} - \tau_{39} + \tau_{40} - \tau_{41})/\sqrt{2}$
33	t R assym	$(-\tau_{37} + 2\tau_{38} - \tau_{39} - \tau_{40} + 2\tau_{41} - \tau_{42})/\sqrt{12}$

C-H Vibrations

The four hydrogen atoms left around the ring in PFBN give rise to four C-H stretching, four C-H in-plane bending and four C-H out-of-plane bending vibrations. The hetroatomic structure shows the presence of C-H stretching vibrations in the region 3100-3000 cm^{-1} , which is the characteristic region for ready identification of C-H stretching vibrations [14]. In this region, the bands are not affected appreciably by the nature of substitutions [15]. Hence, the bands observed at 3086, 3073, 3057, 3000 cm^{-1} in IR and 3087 cm^{-1} in Raman spectrum are assigned to C-H stretching vibrations of the title compound. The C-H in-plane and out-of-plane bending vibrations of the title compounds have also been identified and listed in Table.4.

Table 4: The observed FTIR, FT-Raman and calculated (Unscaled and Scaled) frequencies (cm⁻¹), and probable assignments (characterized by TED) of PFBN using HF/6-311++G(d,p) and B3LYP/6-311++G(d,p) calculations

Symm species C _s	Observed wave numbers (cm ⁻¹)		HF/6-311++G(d,p)						B3LYP/6-311++G(d,p)						TED% among types of coordinates
	FTIR	FT Raman	Un scaled	Scaled	Reduced mass	Force Constants	IR intensity	Raman active	Un scaled	Scaled	Reduced mass	Force Constants	IR intensity	Raman active	
A'	3086 (ms)	3087 (s)	3384	3091	1.0981	7.4102	0.8026	224.0526	3217	3092	1.0966	6.6882	0.8415	247.4393	vCH (99)
A'	3073 (ms)	-	3383	3079	1.0971	7.3981	1.3791	27.5924	3215	3079	1.0953	6.6745	1.0459	28.6439	vCH (98)
A'	3057 (w)	-	3359	3052	1.0928	7.2674	2.0473	68.57911	3195	3055	1.0905	6.5620	2.1432	75.6218	vCH (95)
A'	3000 (w)	-	3358	3006	1.0926	7.2627	2.9887	20.6301	3195	3005	1.0909	6.5617	2.0718	19.221	vCH (92)
A'	2238 (vs)	2238 (vs)	2505	2242	12.6665	46.8568	54.1232	315.7848	2266	2243	12.6551	38.2987	37.6534	450.1030	vCN (88)
A'	1653 (w)	-	1788	1658	5.4450	10.2666	51.0546	60.7850	1637	1658	5.4660	8.6377	46.3722	87.3046	vCC (85)
A'	1607 (vs)	1607 (s)	1761	1610	6.7486	12.3418	7.7635	5.4151	1620	1612	6.7716	10.4773	4.8410	3.1183	vCC (84)
A'	1596 (w)	-	1674	1591	2.3896	3.9469	112.6863	4.0928	1543	1597	2.2853	3.2078	84.2966	5.8291	vCC (82)
A'	1586 (w)	-	1550	1586	2.6074	3.6923	2.6732	0.9341	1440	1583	2.7204	3.3236	2.4141	1.1505	vCC (80)
A'	1511 (vs)	1510(vw)	1457	1516	1.2879	1.6109	1.9213	1.2058	1354	1517	1.3115	1.4184	1.8982	1.6222	vCC (81)
A'	1409 (ms)	-	1335	1415	2.9027	3.0516	77.5060	5.4086	1326	1414	9.7942	10.1545	3.3773	1.3319	vCC (79)
A'	1307 (vs)	-	1311	1312	7.7189	7.8213	13.1933	3.1528	1228	1315	1.7481	1.5537	28.081	5.2870	vCC (78)
A'	1294 (ms)	-	1302	1290	5.6754	5.6766	3.7280	44.4825	1221	1291	4.8739	4.2853	6.4635	46.3148	vCF (75)
A'	1280 (vs)	-	1289	1286	1.2520	1.2258	34.5777	7.3133	1189	1285	1.8970	1.5810	83.2506	21.7820	bCH (70)
A'	1243 (ms)	-	1209	1248	1.4903	1.2838	1.8965	2.1667	1138	1245	1.3750	1.0500	6.8693	0.8952	bCH (74)
A'	-	1220(ms)	1129	1226	1.3863	1.0427	0.0000	0.0030	1046	1225	2.7159	1.7534	5.6097	0.2090	bCH (72)
A'	1198 (w)	-	1124	1193	2.7061	2.0144	4.8621	0.0360	1006	1195	1.3710	0.8178	0.0000	0.0131	bCH (71)
A'	-	1180(ms)	1089	1185	1.3459	0.9415	0.6787	0.5438	980	1186	1.3020	0.7369	0.6990	0.4447	bCN (70)
A'	1167 (w)	-	969	1172	1.6198	0.8962	116.5423	0.1934	870	1183	1.6116	0.7199	92.7483	0.0805	bCCC (69)
A'	-	1100 (w)	955	1105	1.2419	0.6675	0.0000	0.0076	853	1105	1.2422	0.5331	0.0000	0.0551	bCCC (67)
A'	947 (vs)	950 (w)	898	951	6.7668	3.2199	9.6376	37.8047	837	953	6.8434	2.8262	11.1390	35.3398	bCCC (68)
A'	-	860 (s)	800	866	4.1397	1.5625	2.3434	4.4515	726	865	4.4223	1.3766	1.7159	2.4033	bCCC (65)
A''	837 (ms)	-	737	833	6.7947	2.1754	30.5749	0.4917	686	836	6.9110	1.9166	28.2864	0.3548	ωCH (64)
A''	815 (vs)	810 (w)	724	819	7.4348	2.2965	0.0140	3.1851	670	821	7.3955	1.9602	0.0000	4.4135	ωCH (62)
A''	708 (w)	705 (w)	641	713	3.2065	0.7771	23.1572	3.6855	577	712	3.2787	0.6439	20.1245	1.8034	ωCH (63)
A''	687 (w)	-	632	692	7.4677	1.7580	0.2338	6.6105	574	691	7.3854	1.4349	0.0816	3.2403	ωCH (60)
A'	-	670 (ms)	522	675	4.7079	0.7579	1.2683	5.4034	470	676	4.8229	0.6283	1.3238	3.8080	bCF (64)
A''	644 (w)	-	474	640	2.8270	0.3744	0.0000	0.0000	429	644	2.8926	0.3146	0.0000	0.0021	ωccc (60)
A''	-	570 (w)	445	575	12.8289	1.4984	1.5721	6.8578	416	576	12.9246	1.3215	2.5030	7.5461	ωccc (61)
A''	-	550 (w)	421	555	6.8888	0.7228	3.7771	0.5236	384	554	7.0198	0.6113	2.7542	0.5967	ωccc (59)
A''	544 (vs)	-	299	549	8.3165	0.4396	0.0130	0.0394	268	550	8.3921	0.3578	0.0001	0.1079	ωccc (59)
A''	-	471 (ms)	178	477	8.9319	0.1684	10.0380	4.1053	161	476	9.0314	0.1380	8.1176	4.1176	ωCN (60)
A''	-	412 (w)	119	417	10.9844	0.0917	7.9953	0.4507	107	418	10.9412	0.0739	6.8815	0.4248	ωCF (58)

Abbreviations: γ -stretching; b-bending; ω -out-of-plane bending; R-ring; trigd-trigonal deformation; symd-symmetric deformation; asymd-antisymmetric deformation; t-torsion; s-strong; vs-very strong; ms-medium strong; w-weak; vw-very weak.

C-N Vibrations

For the aromatic compound which bears a C=N group attached to the ring, a band of very good intensity has been observed in the region 2240-2221 cm⁻¹ and it is being attributed to C=N stretching vibrations [16]. The strong bands obtained at 2238 cm⁻¹ in both IR and Raman spectra are assigned to C=N stretching vibration and the corresponding force constant contribute 88% to the TED.

The in-plane and out-of-plane bending modes of C=N group are strongly coupled with C-C-C bending modes. They are due to the out-of-plane aromatic ring deformation with in plane deformation of the C=N vibration and in- plane bending of the aromatic ring with the C - C = N bending. The FT-Raman band at 1180 and 471 cm⁻¹ are assigned to the individual in-plane and out-of-plane deformation of C=N vibration, respectively for PFBN.

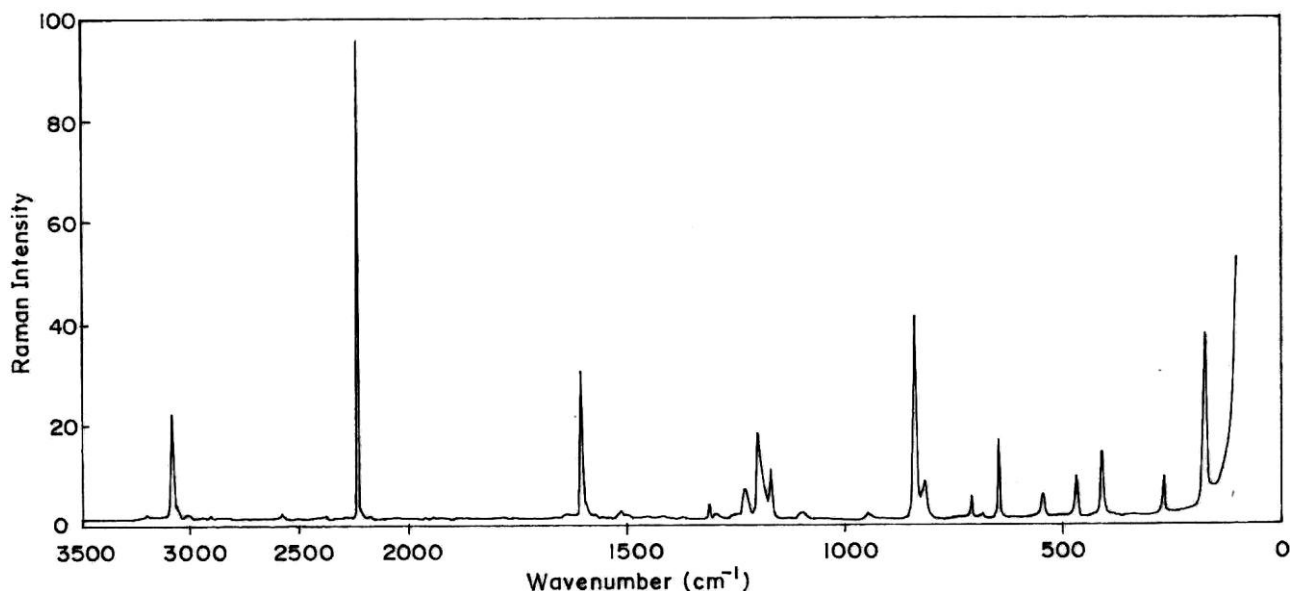


Figure 3: FT-Raman spectrum of P-fluorobenzonitrile

C - F Vibrations

In the vibrational spectra of related compounds, the bands due to C-F stretching vibrations [17] may be found over a wide frequency range 1360-1000 cm^{-1} since the vibration is easily affected by adjacent atoms or groups. In the present investigation, the FTIR band observed at 1294 cm^{-1} has been assigned to C-F stretching mode of vibration for PFBN.

C-C Vibrations

The ring stretching vibrations are very much prominent in the spectrum of pyridine and its derivatives and are highly characteristic of aromatic ring itself [18]. There are very wide fluctuations in intensity [18] in the absorption bands due to aromatic structures in the 1600-1500 cm^{-1} region. In this study the bands between 1607 -1307 cm^{-1} and 1607, 1510 cm^{-1} in FTIR and FT- Raman spectra of PFBN respectively. The higher percentage of total energy distribution (TED) obtained for this group encouraging and confirms the assignments proposed in this study for C-C stretching vibrations of PFBN.

4.3 Vibrational Contribution to NLO Activity and First Hyperpolarizability

The potential application of the title compound in the field of nonlinear optics demands the investigation of its structural and bonding features contributing to the hyperpolarizability enhancement, by analyzing the vibrational modes using IR and Raman spectroscopy. The first hyperpolarizability (β) of this novel molecular system is calculated using the *ab-initio* quantum mechanical method, quantum mechanical method, based on the finite-field approach. In the presence of an applied electric field, the energy of a system is a function of the electric field. The first hyperpolarizability is a third-rank tensor that can be described by a $3 \times 3 \times 3$ matrix. The 27 components of the 3D matrix can be reduced to 10 components due to the Kleinman symmetry [19].

The components of β are defined as the coefficients in the Taylor series expansion of the energy in the external electric field. When the electric field is weak and homogeneous, this expansion becomes

$$E = E_0 - \sum_i \mu_i F^i - \frac{1}{2} \sum_{ij} \alpha_{ij} F^i F^j - \frac{1}{6} \sum_{ijk} \beta_{ijk} F^i F^j F^k - \frac{1}{24} \sum_{ijkl} \nu_{ijkl} F^i F^j F^k F^l + \dots$$

where E_0 is the energy of the unperturbed molecule; F^i is the field at the origin; and μ_i , α_{ij} , β_{ijk} and ν_{ijkl} are the components of dipole moment, polarizability, the first hyperpolarizabilities and second hyperpolarizabilities, respectively. The calculated total dipole moment (μ) of the compound PFBN is 2.402 Debye. The calculated mean first hyperpolarizability (β) of the compound PFBN is 3.1208×10^{-30} esu. The large value of hyperpolarizability, β which is a measure of the non-linear optical activity of the molecular system, is associated with the intramolecular charge transfer, resulting from the electron cloud movement through π conjugated frame work from electron donor to electron acceptor groups. So, we conclude that, the title compound is an attractive object for future studies of nonlinear optical properties.

4.4 Homo-Lumo Analysis

The interaction of two atomic (or) molecular orbitals produces two new orbital. One of the new orbitals is higher in energy than the original ones (the anti bonding orbital) and one is lower (the bonding orbital). When one of the initial orbitals is filled with a pair of electrons (a Lewis base) and the other is empty (a Lewis acid), we can place the two electrons into the lower, energy of the two new orbitals. The "filled-empty" interaction therefore is stabilizing. When we are dealing with interacting molecular orbitals, the two that interact are generally the highest energy occupied molecular orbital (LUMO) of the molecule. These orbitals are the pair of orbitals in the molecule, which allows them to interact most strongly. These orbitals are sometimes called the frontier orbitals, because they lie at the outermost boundaries of the

electrons of molecule. The HOMO-LUMO analysis for the title molecule has been carried out using B3LYP/6-311++G(d,p) level. The HOMO, LUMO plot is shown in the figure 4. The calculated energies of HOMO and LUMO are -5.478 eV and -8.08 eV and the HOMO-LUMO energy gap is found to be 2.53 eV. It shows that the HOMO-LUMO energy gap is low and is responsible for the NLO activity of the molecule.

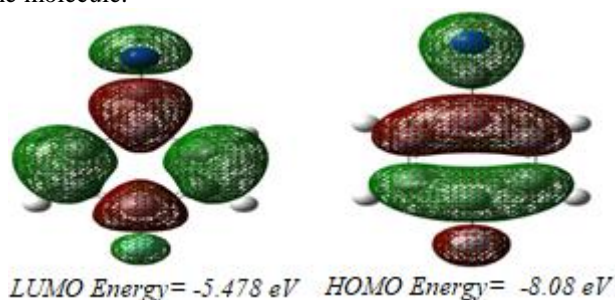


Figure 4: HOMO LUMO plot of PFBN

5. Conclusion

Based on the SQM force field obtained by *ab initio* / HF and DFT/B3LYP methods with 6-311++G(d,p) basis set, a complete vibrational properties of the title compound have been investigated by FTIR and FT-Raman spectroscopies. The various modes of vibrations were unambiguously assigned based on the results of the TED output obtained from normal coordinate analysis. The assignment of the fundamentals is confirmed by the qualitative agreement between the calculated and observed band intensities and polarization properties as well and is believed to be unambiguous. The results confirm the ability of the methodology applied for interpretation of the vibrational spectra of the title compound in solid phase. HOMO and LUMO energy gap explains the eventual charge transfer interactions taking place within the molecule. NLO property has also been observed by predicting the first hyperpolarizability for the title molecule due to the substitution in the benzene.

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