FTIR, FT – Raman and DFT calculations of 2-bromo-6-chloro-4-fluoroaniline

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The Fourier transforms infrared (FTIR) and FT-Raman spectra of 2-bromo-6-chloro-4-fluoroaniline has been measured in the range 4000-400 and 3500-50 cm^{-1} respectively. Utilizing the observed FTIR and FT-Raman data, complete vibrational assignment and analysis of the fundamental modes of the compound was carried out by employing the HF/6-31G(d,p) and B3LYP/6-31G(d,p) methods for optimized geometries. The total energy disyribution (TED) values obtained reflect the correctness of the vibrational assignments.

Key word : FTIR, FT-Raman spectra,2-bromo-6-chloro-4-fluoroaniline, *ab initio*, DFT.

1.   INTRODUCTION

Aniline and its derivatives have been widely used as starting materials in a vast amount of chemicals, pharmaceuticals, dyes, electro-optical and many other industrial processes[1-4]. The conducting Polymer of aniline namely polyaniline is used in microelectronic devices as diodes and transistors[5-8]. Particularly, aniline and its derivatives are used in the production of dyes, pesticides and antioxidants.   Consideration of these factors leads to undertake the detailed spectral investigation of 2-bromo-6-chloro-4-fluoro aniline (BCFA).

2.   EXPERIMENTAL DETAILS

The fine polycrystalline samples of BCFA was obtained from Lancaster Chemical Company, UK and used as such for spectral measurements. The room temperature Fourier transform infrared spectra of the title compound were measured in the region 4000 - 400 cm^{-1} at a resolution of ± 1 cm^{-1}

using KBr pellets on BRUKER IFS - 66V FTIR spectrophotometer equipped with a cooled MCT detector. Boxcar apodization was used for the 250 averaged interferogrames collected for both the sample and background.

The FT - Raman spectra were recorded on a computer interfaced BRUKER IFS model interferometer equipped with FRA 106 FT - Raman accessory in the 3500 - 50 cm^{-1} Stoke's region using the 1064 nm line of a Nd:YAG laser for excitation operating at 200 mW power. The reported wavenumbers are believed to be accurate within ± 1 cm^{-1}.

3. COMPUTATIONAL DETAILS

The assignments of band in the vibrational spectra of molecule are an essential step in application of vibrational spectroscopy for solving various structural and chemical problems. For the better understanding of IR and Raman spectra, reliable assignments of all vibrational bands are essential. Recently, Density Functional Theory (DFT)[9] has been accepted by *ab initio* quantum chemistry community as a cost effective general procedure for studying physical properties of the molecules. In the present study, owing to the industrial importance of substituted anilines, an extensive spectroscopic studies of BCFA has been undertaken by recording FTIR and FT-Raman spectra and subjecting them to normal coordinate analysis, in an effort to provide possible explanations for the experimentally observed vibrational fundamentals and to understand the effect of halogen and methyl group substitution on the characteristic frequencies of the amino group. In order to obtain the optimized structural parameters, vibrational frequencies, minimum energy, reduced mass, force constants, IR intensity and Raman activity, have been carried out by applying the *ab initio* and DFT calculation. These calculations were carried out using the GAUSSIAN 03W software package at the HF (Hartree- Fock) and B3LYP (Becke-3-Lee-Yang-Parr) level with 6-31G+ (d, p) basis set. Since the recent studies have shown that the combination of vibrational spectroscopy

with *ab initio* calculations can be a powerful tool for understanding the fundamental modes of vibrations of the molecules.

4. RESULTS AND DISCUSSION

4.1. Molecular geometry

The optimized molecular structure of BCFA having C_s point group symmetry are shown in Fig. 1. The global minimum energy obtained by the HF and DFT structure optimization for BCFA is calculated as -3412.79543216 Hartrees and -3417.53192112 Hartrees. The optimizated geometrical parameters obtained by the large basis set calculations in this study for BCFA are presented in Table.1.

4.2. Symmetry coordinates

Detailed description of vibrational modes is given by means of normal coordinates analysis. For this purpose, the full set of 48 standard internal valences coordinates (containing 12 redundancies) for defined as given in Table 2. From this, a non redundant set of local symmetry coordinates were constructed (Table 3) and much like 'natural internal coordinates recommended[10,11] by IUPAC. Theoretically calculated force fields were transforming to this later set of vibrational coordinates and used in all subsequent calculations.

4.3 Vibrational Spectra

The title compounds consists of 14 atoms and its 36 normal modes are distributed amongst the symmetry species as:

$$\overline{3N} - 6 = 25 \ A' \ (\text{in-plane}) + 11 \ A'' \ (\text{out-of-plane})$$

All the vibrations are active both in IR and Raman spectra.

The detailed vibrational band assignments of BCFA calculated by the *ab initio* and DFT calculations based on HF and B3LYP level with 6-31+G (d,p) basis set along with the calculated IR and Raman intensities and normal mode descriptions (Characterised by TED) are reported in Table 4. The FTIR and FT-Raman spectra of BCFA are shown in Figs.2 & 3.

4.4. Vibrational band assignments

IR and Raman spectra contain a number of bands at specific wavenumbers. The aim of the vibrational analysis is to decide which of the vibrational modes give rise to each of these observed bands. In the present study, the vibrational spectra of the title compound has been interpreted on the basis of normal coordinates analysis and force field calculations.

C - H Vibrations

The C-H stretching vibrations of aromatic and heteroaromatic structure[12,13] are normally appearing in the region 3000 - 3100 cm^{-1}. In this region, the bands are not affected appreciably by the nature of the substituent. Hence, in the present investigation, the C–H stretching vibrations of BCFA are observed at 3083 cm^{-1} in both IR and Raman and 2929 cm^{-1} in IR spectrum. The bands observed at 3082,   3083 cm^{-1} in both IR and Raman and 2989 cm^{-1} in FT-Raman have been designated to C-H stretching vibrations for BDCA. The C-H in-plane and out-of-plane bending vibrations of the title compounds have also been identified and listed in Table 4.

C - C Vibrations

The bands between 1400 and 1650 cm^{-1} in benzene derivatives are due to C-C stretching vibrations[16]. Therefore, the stretching vibrations of BCFA are observed at 1612, 1553, 1402 cm^{-1} in Raman and 1574, 1472, 1413 cm^{-1} in FTIR spectrum.   The C-C stretching vibrations of BDCA are observed between 1561-1445 cm^{-1} and 1611 – 1467 cm^{-1} in FTIR and FT-Raman spectrum, respectively. The in-plane and out-of-plane bending vibrations of carbon - carbon group are presented in Table 4.

C - F Vibrations

In the vibrational spectra of related compounds, the bands due to C-F stretching vibrations[15] 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 FT-Raman band observed at 1301 cm^{-1} has been assigned to C-F stretching mode of vibration.

C - Cl Vibrations

The C-Cl stretching frequency is generally observed in the region 800-600 cm^{-1} depending upon the configuration and conformation of the compound[16]. Based on this, in the present study, the FTIR band of BCFA identified at 846 cm^{-1} is assigned to C-Cl stretching mode of vibration.   The in-plane and out-of-plane vibrational modes are given in Table 4 for the title compound.

C - Br Vibrations

The assignment of C - Br stretching and deformation modes have been made through comparison with assignments in other halogens substituted benzene   derivatives[17]. Krishnakumar et al.,[18,19] have assigned the C-Br vibrations in the frequency range 1300-550 cm^{-1}. In this study, the band observed at 562 cm^{-1} in FTIR spectrum and 552 cm^{-1} in both IR, Raman have been designated to C-Br stretching.

NH$_2$ Group Vibrations

The frequencies of amino group appear around 3500 - 3300 cm^{-1} for NH$_2$ stretching, 1700-1600 cm^{-1} for scissoring and 1150 - 900 cm^{-1} for rocking deformation[17]. In the present study, the asymmetric and symmetric stretching modes of NH$_2$ group in BCFA are assigned at 3444 cm^{-1} in IR and 3365 cm^{-1} in Raman spectra.   The bands appeared at 1627 cm^{-1} in IR have been assigned to scissoring modes of NH$_2$ group . The Rocking, wagging and twisting vibrational modes of NH$_2$ for the title compounds are also presented in Table 4.

5. CONCLUSION

The molecular structural parameters and fundamental vibrational frequencies of the optimised geometry of 2-bromo-6-chloro-4-fluoroaniline has been obtained from *ab initio* and DFT calculations. The effect of substituent (bromo, chloro and fluoro,) on vibrational frequencies is analysed in detail. The assignments of most of the fundamentals provided in the present work are believed to be unambiguous. The TED calculation regarding the normal modes of vibration provides a strong support for the frequency assignment.
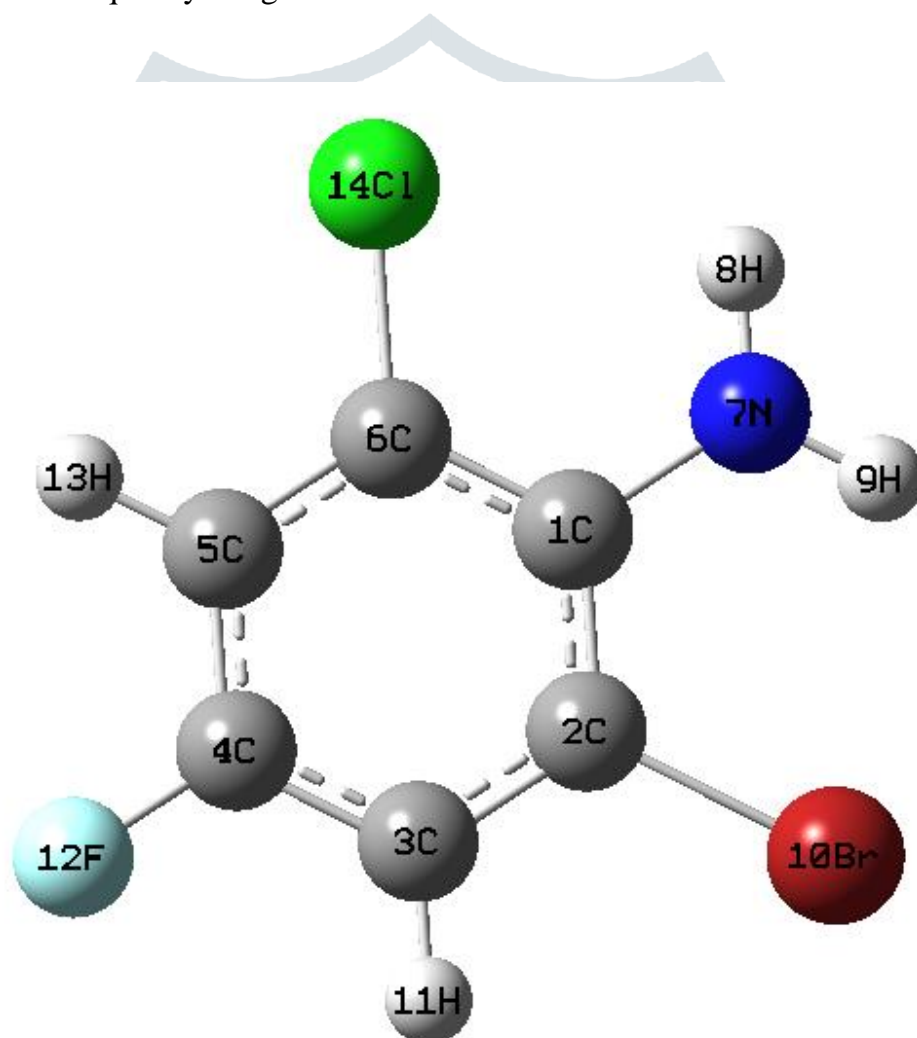

Fig. 1 Molecular structure of 2-bromo-6-chloro-4-fluoroaniline

Table 1

Optimized geometrical parameters of 2-bromo-6-chloro-4-fluoroaniline obtained by B3LYP/6-31+G (d,p) and HF/6-31+G (d,p) density functional calculations

Bond length	Value (Å)		Bond angle	Value (Å)	
	B3LYP/ 6-31G+(d,p)	HF/ 6-31G+(d,p)		B3LYP/ 6-31G+(d,p)	HF/ 6-31G+(d,p)
$C_1 - C_2$	1.4068	1.3968	$C_1 - C_2 - C_3$	122.5035	122.8026
$C_2 - C_3$	1.3938	1.3812	$C_2 - C_3 - C_4$	118.2759	118.6756
$C_3 - C_4$	1.3875	1.3735	$C_3 - C_4 - C_5$	118.9032	121.3739
$C_4 - C_5$	1.3884	1.3743	$C_4 - C_5 - C_6$	117.5726	118.7077
$C_5 - C_6$	1.3922	1.3802	$C_5 - C_6 - C_1$	123.2254	122.7622
$C_6 - C_1$	1.4088	1.3982	$C_6 - C_1 - C_2$	116.063	115.6777
$C_1 - N_7$	1.4244	1.3771	$C_6 - C_1 - N_7$	123.6866	121.8310
$N_7 - H_8$	1.0177	0.9935	$C_2 - C_1 - N_7$	120.2503	122.4449
$N_7 - H_9$	1.0177	0.9934	$H_8 - N_7 - H_9$	106.3076	113.9705
$C_2 - Br_{10}$	1.9021	1.8991	$C_1 - C_2 - Br_{10}$	119.6743	119.4414
$C_3 - H_{11}$	1.0823	1.0722	$C_3 - C_2 - Br_{10}$	117.8222	117.7560
$C_4 - F_{12}$	1.3455	1.3296	$C_2 - C_3 - H_{11}$	121.4241	121.0094
$C_5 - H_{13}$	1.0825	1.0725	$C_4 - C_3 - H_{11}$	120.3000	120.3149
$C_6 - H_{14}$	1.7575	1.7442	$C_3 - C_4 - F_{12}$	118.9032	119.3581
			$C_5 - C_4 - F_{12}$	118.7373	119.2679
			$C_4 - C_5 - H_{13}$	120.6734	120.4363
			$C_6 - C_5 - H_{13}$	121.7540	120.8560
			$C_5 - C_6 - H_{14}$	118.0488	117.9948
			$C_1 - C_6 - H_{14}$	118.7259	119.2431
			$C_1 - N_7 - H_9$	110.4491	116.0779
			$C_1 - N_7 - H_8$	110.4491	115.8495

For numbering of atoms refer Fig. 1

Table 2

Definition of internal coordinates of 2-bromo-6-chloro-4-fluoroaniline

No. (i)	Symbol	Type	Definition[a]
Stretching			
1 – 2	r_i	C-H	$C_3 - H_{11}$, $C_5 - H_{13}$
3	R_i	C-F	$C_4 - F_{12}$
4	Q_i	C-Br	$C_2 - Br_{10}$
5	q_i	C-Cl	$C_6 - Cl_{14}$
6	S_i	C-N	$C_1 - N_7$
7 – 12	P_i	C-C	$C_1 - C_2$, $C_2 - C_3$, $C_3 - C_4$, $C_4 - C_5$, $C_5 - C_6$, $C_6 - C_1$
13, 14	T_i	N-H	$N_7 - H_8$, $N_7 - H_9$
In-plane bending			
15 – 20	β_i	C-C-C	$C_1 - C_2 - C_3$, $C_2 - C_3 - C_4$, $C_3 - C_4 - C_5$, $C_4 - C_5 - C_6$, $C_5 - C_6 - C_1$, $C_6 - C_1 - C_2$
21 – 24	α_i	C-C-H	$C_6 - C_5 - H_{13}$, $C_4 - C_5 - H_{13}$, $C_4 - C_3 - H_{11}$, $C_2 - C_3 - H_{11}$
25, 26	ν_i	C-C-F	$C_5 - C_4 - F_{12}$, $C_3 - C_4 - F_{12}$
27, 28	π_i	C-C-Br	$C_1 - C_2 - Br_{10}$, $C_3 - C_2 - Br_{10}$
29, 30	ϕ_i	C-C-Cl	$C_5 - C_6 - Cl_{14}$, $C_1 - C_6 - Cl_{14}$
31, 32	σ_i	C-C-N	$C_6 - C_1 - N_7$, $C_2 - C_1 - N_7$
33, 34	ε_i	C-N-H	$C_1 - N_7 - H_8$, $C_1 - N_7 - H_9$
35	δ_i	H-N-H	$H_8 - N_7 - H_9$
Out-of-plane bending			
36, 37	ψ_i	C-H	$H_{11} - C_3 - C_4 - C_2$, $H_{13} - C_5 - C_6 - C_4$
38, 39	ρ_i	C-F	$F_{12} - C_4 - C_5 - C_3$
40	χ_i	C-Br	$Br_{10} - C_2 - C_1 - C_3$
41	ω_i	C-N	$N_7 - C_1 - C_6 - C_2$
Torsion			
42 – 47	τ_i	t Ring	$C_1 - C_2 - C_3 - C_4$, $C_2 - C_3 - C_4 - C_5$, $C_3 - C_4 - C_5 - C_6$, $C_4 - C_5 - C_6 - C_1$, $C_5 - C_6 - C_1 - C_2$, $C_6 - C_1 - C_2 - C_3$
48	τ_i	t C-NH$_2$	$C_1 - N_7 - H_8 - H_9$

[a]For numbering of atoms refer Fig. 1

Table 3

Definition of local symmetry coordinates of 2-bromo-6-chloro-4-fluoroaniline

| No. (i)	Type	Definition
1, 2	C H	r_1, r_2
3	C F	R_3
4	C Br	Q_4
5	C Cl	q_5
6	C N	S_6
7 – 12	C C	$P_7, P_8, P_9, P_{10}, P_{11}, P_{12}$
13	NH$_2$ ss	$(T_{13} + T_{14}) / \sqrt{2}$
14	NH$_2$ ass	$(T_{13} - T_{14}) / \sqrt{2}$
15	R trigd	$(\beta_{15} - \beta_{16} + \beta_{17} - \beta_{18} + \beta_{19} - \beta_{20}) / \sqrt{6}$
16	R symd	$(-\beta_{15} - \beta_{16} + 2\beta_{17} - \beta_{18} - \beta_{19} - 2\beta_{20}) / \sqrt{12}$
17	R asymd	$(\beta_{15} - \beta_{16} + \beta_{18} - \beta_{19}) / 2$
18, 19	b C H	$(\alpha_{21} - \alpha_{22}) / \sqrt{2}$, $(\alpha_{23} - \alpha_{24}) / \sqrt{2}$
20	b C F	$(\nu_{25} - \nu_{26}) / \sqrt{2}$
21	b C Br	$(\pi_{25} - \pi_{28}) / \sqrt{2}$
22	b C Cl	$(\phi_{29} - \phi_{30}) / \sqrt{2}$
23	b C N	$(\sigma_{31} - \sigma_{32}) / \sqrt{2}$
24	NH$_2$ twist	$(\varepsilon_{33} - \varepsilon_{34}) / \sqrt{2}$
25	NH$_2$ rock	$(\varepsilon_{33} + \varepsilon_{34}) / \sqrt{2}$
26	NH$_2$ sciss	$(2\delta_{35} - \varepsilon_{33} - \varepsilon_{34}) / \sqrt{6}$
27, 28	ω C H	ψ_{36}, ψ_{37}
29	ω C Cl	μ_3
30	ω C F	ρ_{39}
31	ω C Br	χ_{40}
32	C N	ω_{41}
33	Ring trigd	$(\tau_{42} - \tau_{43} + \tau_{44} - \tau_{45} + \tau_{48} - \tau_{47}) / \sqrt{6}$
34	Ring symd	$(\tau_{42} - \tau_{44} + \tau_{45} - \tau_{47}) / \sqrt{2}$
35	Ring asymd	$(-\tau_{42} + 2\tau_{43} - \tau_{44} - \tau_{45} + 2\tau_{46} - \tau_{47}) / \sqrt{12}$
36	t C-NH$_2$ wag	τ_{48}

Table 4.
Assignment of fundamental vibrational modes of 2-bromo-6-chloro-4-fluoroaniline by normal mode analysis based on SQM force field calculations using selectively scaled B3LYP/6-31+G(d,p) and HF/6-31+G(d,p) force field.

Symmetry species C_s	Observed frequencies (cm^{-1})		Calculated frequencies (cm^{-1}) (Unscaled)		Scaling frequency (cm^{-1})	Reduced mass (AMU)		Force constant (mDyne/A)		IR intensity (KM/Mole)		Raman activity (A^4/AMU)		Assignment (% TED)
	FTIR	FT-Raman	B3LYP	HF		B3LYP 6-31+G(d,p)	HF 6-31+G(d,p)	B3LYP 6-31+G(d,p)	HF 6-31+G(d,p)	B3LYP 6-31+G(d,p)	HF 6-31+G(d,p)	B3LYP 6-31+G(d,p)	HF 6-31+G(d,p)	
A'	3444(vs)	-	3567	3951	3446	1.0589	7.1722	0.0533	0.0457	46.5548	1.1252	1.9228	0.5158	NH$_2$ ass (99)
A'		3365(w)	3494	3834	3369	6.7523	16.9532	0.0376	0.3545	0.5481	0.0823	0.2346	1.7289	NH$_2$ ss (98)
A'	3083(w)	3083(s)	3244	3405	3081	17.3029	8.8504	0.2928	0.2000	0.0378	0.7744	1.9344	0.8875	ν CH (97)
A'	2929(w)	-	3243	3403	2927	8.3936	3.9428	0.1490	0.1174	0.0024	1.2916	0.3117	2.8587	ν CH (96)
A'	1627(ms)	-	1663	1831	1623	4.7941	19.1717	0.1185	0.7214	0.7405	0.0798	1.8518	2.4565	NH$_2$ sciss (89)
A'	-	1612(vw)	1644	1799	1616	17.3429	2.8910	0.5650	0.1539	0.3710	2.0803	2.1509	1.5131	ν CC (78)
A'	1574(ms)	-	1602	1773	1572	6.9293	1.7841	0.3250	0.1158	4.9412	15.1224	1.2574	3.3668	ν CC (82)
A'	-	1553(vw)	1501	1634	1550	10.4026	3.8384	0.7151	0.3213	0.3388	5.8283	4.3125	3.4929	ν CC (80)
A'	1472(ms)	-	1422	1567	1474	4.9367	4.9763	0.3810	0.5188	3.0733	25.0309	2.7930	1.3930	ν CC (79)
A'	1413(w)	-	1319	1439	1420	7.2084	7.2312	0.8148	0.9512	8.2034	2.5820	3.0952	3.5893	ν CC (76)
A'	-	1402(vw)	1296	1388	1407	10.7189	9.9521	1.4271	1.5626	1.1265	4.1206	9.3666	9.9383	ν CC (74)
A'	-	1388(vw)	1233	1351	1380	5.2251	1.4042	0.9097	0.2684	0.0200	305.3903	0.7911	3.4134	ν CN (72)
A'	-	1301(s)	1222	1240	1300	4.2307	5.3139	0.8134	1.0370	7.8227	0.8356	1.3927	0.1292	ν CF (78)
A'	1296(s)	-	1194	1169	1294	3.8476	3.9207	0.8203	0.8768	0.8488	0.1370	0.0134	0.9976	b CH (81)
A'	1193(s)	-	1071	1159	1195	4.4873	3.3458	1.3766	0.8330	1.4929	2.9081	0.1335	0.0949	b CH (79)
A'	1089(w)	-	958	1029	1094	5.9994	7.2844	2.0706	2.8940	38.4729	24.9260	0.8919	2.0064	R asymd (80)
A'	-	1079(w)	884	1016	1070	6.0673	8.9165	2.2115	3.6072	38.9170	61.0777	11.8648	0.1680	R symd (72)
A'	1053(ms)	-	857	1001	1051	1.5167	5.0009	0.6494	2.1777	180.4590	29.0452	2.3145	10.9564	NH$_2$ rock (76)
A'	-	933(ms)	853	860	932	1.4078	1.4932	0.6088	0.8819	26.6467	43.8688	1.3436	1.2531	R trigd (70)
Symmetry species C_s	Observed frequencies (cm^{-1})		Calculated frequencies (cm^{-1}) (Unscaled)		Scaling frequency	Reduced mass (AMU)		Force constant (mDyne/A)		IR intensity (KM/Mole)		Raman activity (A^4/AMU)		Assignment (% TED)

	FTIR	FT-Raman	B3LYP	HF	(cm⁻¹)	B3LYP 6-31+G(d,p)	HF 6-31+G(d,p)	B3LYP 6-31+G(d,p)	HF 6-31+G(d,p)	B3LYP 6-31+G(d,p)	HF 6-31+G(d,p)	B3LYP 6-31+G(d,p)	HF 6-31+G(d,p)	
A'	929(s)	-	787	829	930	1.4077	1.3564	0.6479	0.8252	14.9722	3.3763	1.4376	0.7553	b CN (75)
A'	846(s)	-	765	821	848	9.6042	8.9294	5.1896	5.5752	45.6732	60.2388	11.5660	7.4457	ν CCl (78)
A'	562(w)	-	722	650	568	2.2812	2.5988	1.5411	2.0571	7.4643	91.8799	4.9588	4.6165	ν CBr (70)
A'	-	476(vs)	602	616	470	1.4979	2.5273	1.2576	2.0356	8.4193	60.0526	1.0252	8.1519	b CF (68)
A'	-	433(w)	571	576	427	1.2694	1.8914	1.1161	1.7136	0.1300	8.4884	1.5406	18.1321	b CCl (65)
A'	-	412(vw)	544	570	410	2.1962	2.2233	1.9664	2.3898	21.7073	31.6464	6.8394	4.0016	b CBr (64)
A"	-	789(ms)	475	516	796	9.4935	1.4235	9.3986	1.6148	14.4510	3.2359	7.6470	2.4521	NH₂ wag (59)
A"	761(ms)	-	438	473	761	9.6626	8.4633	9.9056	10.3231	9.1005	3.8461	15.1108	20.2549	ω CH (60)
A"	706(w)	-	362	421	708	3.7786	4.0464	4.4999	5.8499	29.0370	13.2156	0.2468	0.4479	ω CH (58)
A"	-	689(vw)	342	377	683	5.1964	4.8009	6.8986	7.5540	141.8888	267.9708	0.3409	1.5487	t R asymd (55)
A"	-	651(vw)	282	332	655	4.7429	7.5968	7.1724	14.0627	50.8677	37.0129	10.8770	7.1264	t R trigd (57)
A"	-	602(vw)	235	301	600	5.4756	1.8087	8.7238	3.4476	97.9144	178.4604	16.8159	1.8320	t R symd (58)
A"	-	485(w)	205	253	488	1.3020	2.1731	2.1219	4.2911	69.4586	20.6619	17.9909	18.3419	ω CN (54)
A"	-	402(vw)	174	225	398	1.0931	1.0948	6.7728	7.4709	0.5409	0.6213	103.6561	92.5279	ω CF (53)
A"	-	387(w)	170	196	390	1.0930	1.0949	6.7770	7.4809	2.7188	1.8528	63.9063	63.3215	ω CCl (55)
A"	-	348(vw)	97	188	352	1.0490	1.0479	7.5435	9.0774	7.5427	45.5971	141.9185	86.0398	NH₂ twist (53)
A"	-	235(w)	88	104	230	1.0924	1.1010	8.1891	10.1276	8.5050	44.7121	67.2380	27.1902	ω CBr (52)

Abbreviations: ν - stretching; b - in-plane bending; ω - out-of-plane bending; asymd - asymmetric; symd - symmetric; t - torsion; trig - trigonal; w - weak; vw-very week; vs - very strong; s - strong; ms - medium strong; ss - symmetric stretching; ass - asymmetric stretching; ips - in-plane stretching,; ops - out-of-plane stretching; sb - symmetric bending; ipr - in-plane rocking; opr - out-of-plane rocking; opb - out-of-plane bending
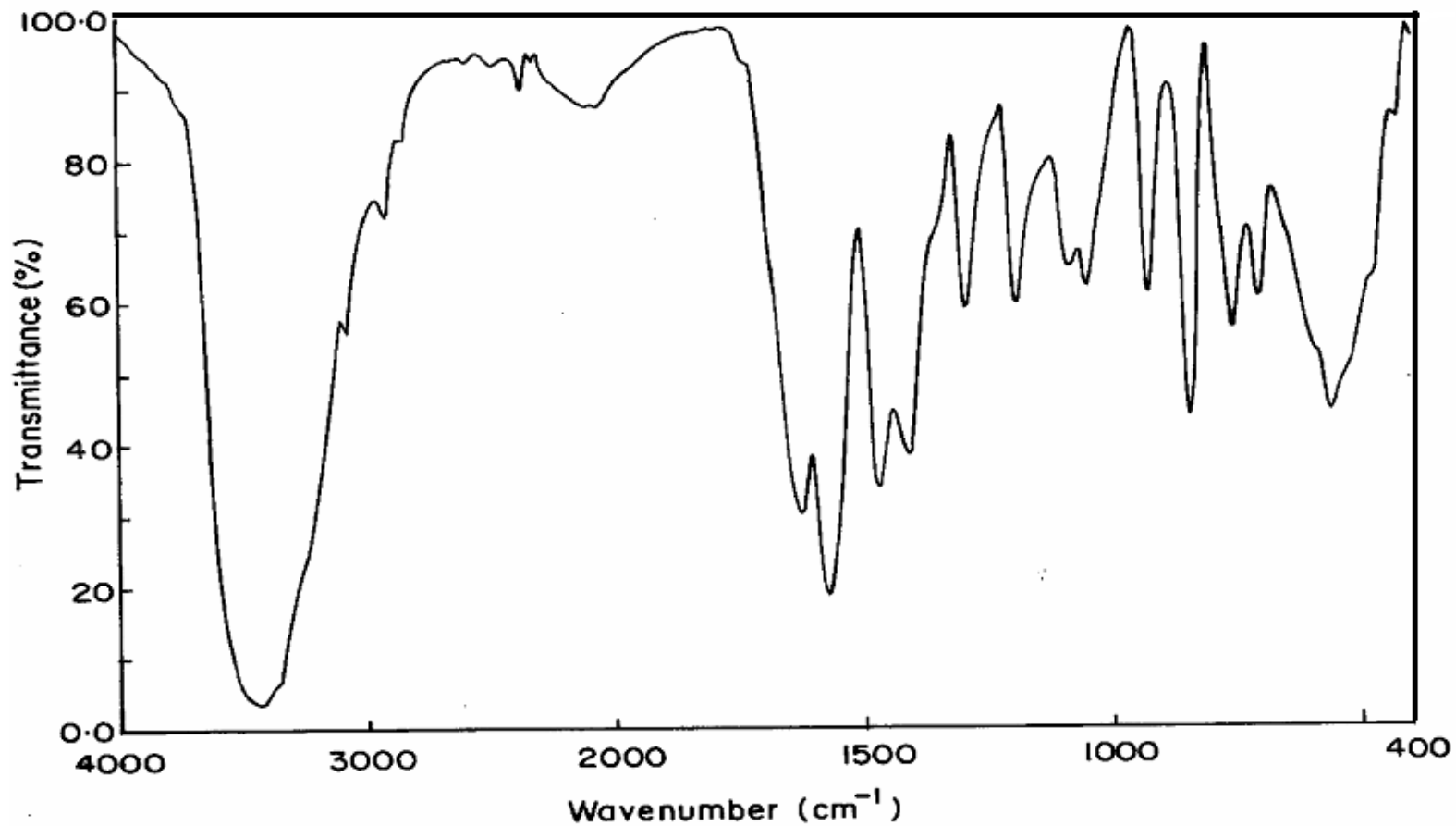
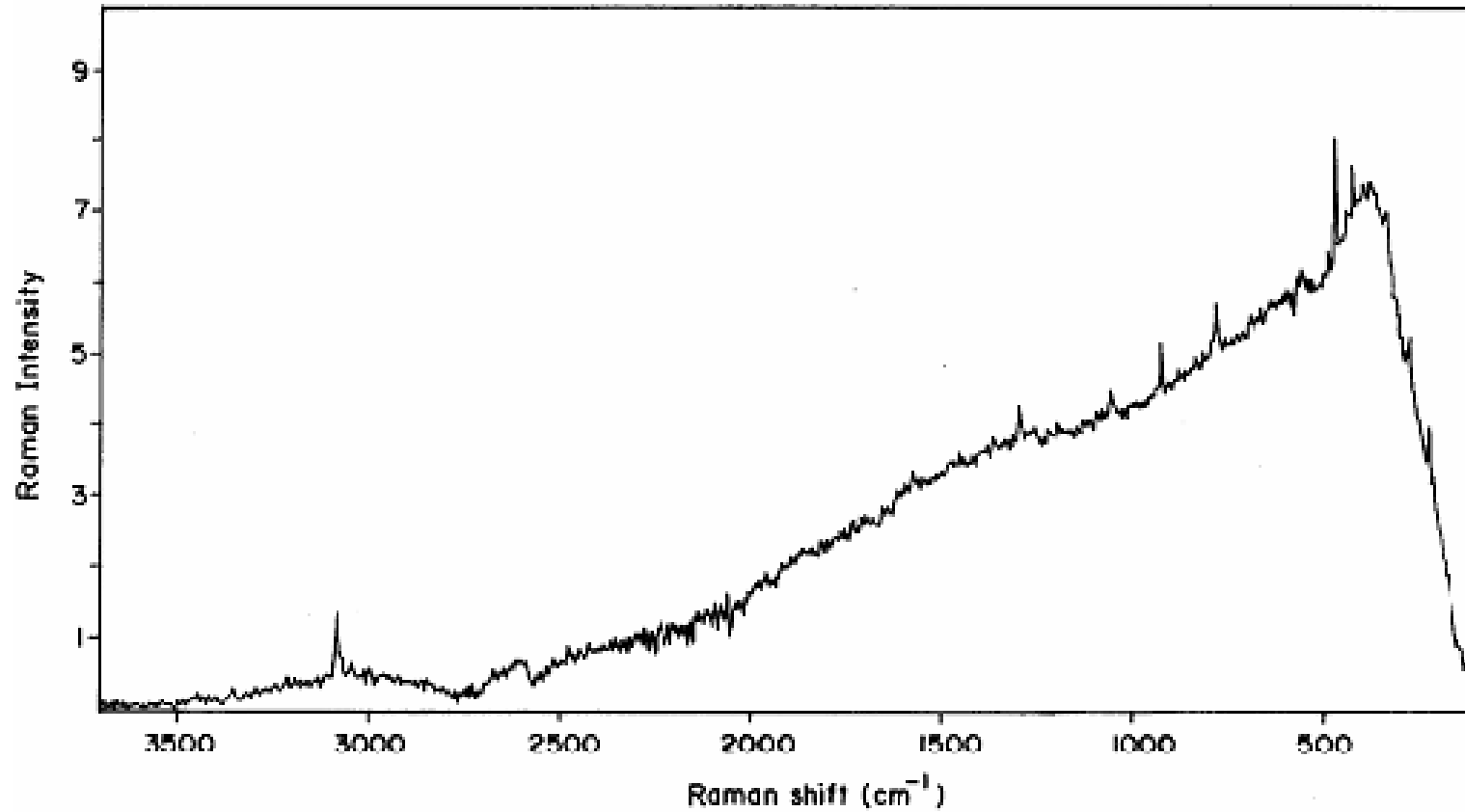. Fig. 2 - FTIR spectrum of 2-bromo-6-chloro-4-fluoroaniline

Fig. 3 - FT-Raman spectrum of 2-bromo-6-chloro-4-fluoroaniline

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