Vibrational Dynamics of 2-[3-(p-flourobenzoyl) Propyl]-1,2,3,4,6,7,12,12, a-octahydropyrazino[2',1':6,1] Pyrido [3,4-b] Indole [centbutindole]: A Potent Nuroleptic Drug

D.B.Singh[1*], Abadur-Rahman[2], V.N.Shukla[3], Vikash Kumar[4] and Pragya Gupta[5]

ABSTRACT

FITR spectra and normal mode analysis of compound 2-[3-(p-flourobenzoyl)propyl]-1,2,3,4,6,7,12,12, a-octahydropyrazino[2',1':6,1] pyrido [3,4-b] indole [centbutindole], which is a potent nuroleptic drug and belong to a series of 2-substituted pyrazino-pyrido indoles. It also blind with $5HT_2$ receptors. It has shown good antihypotensive activity. The well known Wilson's G-F matrix method with Urey-Bradely force field has been used to evaluate the normal mode frequencies of vibration. Good agreement has been obtain between them and a set of 29 force field constants is established. The vibrational dynamics of the title compound is being reported using Urey Bradley force field. It has shown acute toxicity, gross behavior and central effects like anti convulsant activity, anti reserpine activity and stereo specificity of action. The conformation of the title compound was determined by X-ray diffraction. It is planned to determine the conformation in such cases by the application of Fourier Transform Infrared (FITR) spectroscopy and normal mode analysis. As a first step in this direction the FITR spectrum of the title compound has been recorded and its normal mode analysis is carried out. The assignments of the frequencies are based on the theoretically calculated frequencies have also been given their best assignment.

***Keywords**: Vibrational frequencies, FITR spectra, Force constant, IR band assignments, Conformation.*

1. INTRODUCTION

2-[3-(p-flourobenzoyl)propyl]-1,2,3,4,6,712,12 a-octahydropyrazino [2',1':6,1} pyrido [3,4-b] indole (centbutindole)[1-2] is a potent nuroleptic drug has a florobutyrophenone moiety[3-4] and belong to a series of 2- substituted pyrazino –pyrido indoles synthesized for CNS activity[4-6.] It mainly acts as Dopamine D2 receptor[7-9] and $5HT_2$ receptor blocker[10-11].The conformation of a drug molecule plays an important role in drug receptor interactions, which lead to its biological response. Several methods are available which predict such effects[12-15] and provide insight to active site space and binding requirements, but most of these are biased due to arbitrarily chosen molecule overlays on binding site points. The conformation of the title compound was determined by Rusing et al[16] using X-ray diffraction.

The classical neuroleptic agents like Chlorpromazine, Haloperidole[17-18] and fluphenazine are effective in controlling the positive symptoms of schizophrenia presence of altered behaviors, such as delusions , hallucinations, usually auditory[19], extreme

1*. Mr. D.B. Singh - Molecular, Spectroscopy &Bio-physics Laboratory, Global group of Institutions Lucknow (U.P.), India.
2. Mr. Abadur - Rahman - Deptt. of Applied Science & Humanities, Azad group of Technical Campus Lucknow (U.P.), India.

emotion, excited motor activity and incoherent thoughts and speech, these drugs are less efficacious in attenuating negative symptoms[20] a lack of behaviors, such as emotion, speech, social interaction and action and are also associated with side effect including involuntary movement disorders or extra pyramidal side effects (EPS). These negative symptoms of schizophrenia are the primary target for new drugs from an effectiveness stand point[21-26]. The serotonergic $5HT_2$ receptor has been shown to attenuate the negative symptoms of schizophrenia[27-28] and for reducing EPS29. Hence the neuroleptic with right balance of Dopamine D2 and $5HT_2$ receptor antagonism may be important for successful treatment of schizophrenia.

The vibrational dynamics of the title compound centbutindole has been reported using Urey Bradely force field. As a first step in this direction the Fourier Transform Infrared (FTIR)[30] spectrum of the title compound has been recorded and its normal mode analysis is carried out. It is used for variety of other applications[31-35].

The assignments of the frequencies are based on the concept of group frequency, Potential energy distribution and band intensities. The experimentally observed frequencies have been tabulated along with the theoretically calculated ones and their assignments. The well known Wilson's G-F matrix method with Urey-Bradely force field has been used to evaluate the normal mode frequencies of vibration. If the theoretical frequencies agree with those in FTIR spectra, then it is concluded that the calculated geometry is correct; otherwise it is determine again using different procedure for minimization. These verified conformations may then be utilized in establishing the three dimensional quantitative structure-activity relationships4. The X-ray determines structure16 has been utilized in carrying out its normal mode calculations. A set of force field constantans has been established to obtain a good agreement between the theoretical frequencies and the observed spectra. These results are presented in this paper.

2. MATERIAL METHOD AND THEORY

The compound 2-[3-(p-flourobenzoyl) propyl]-1,2,3,4,6,7,12,12a

Octahydropyrazino [2',1',:6,1] pyrido [3,4-b]indole was synthesized from piprazine rigid frame work, as reported in literature[4].

The FTIR spectra in KBr and in dilute $CHCl_3$solution where recorded on the Impact 400 spectrometer Nicolet Co. having a resolution of $1cm^{-1}$ using interferometer dispersing KBr beam splitter and having noise level equal to RMS7.1.The X-ray data used for the calculation were taken from Rusing et al[16].The well-known Wilson's G-F metrics method with Urey-Bradley force field was used to evaluate the normal mode frequencies of vibration. These are given by the Eigen values of the secular equation.

$$GFL=\lambda L \qquad (1)$$

as $$\lambda = 4\pi^2 c^2 f^2 \qquad (2)$$

The potential is represented as

$$V = \sum_{j,k}\{K'_{jk}\nu_{jk}(\Delta\nu_{jk}) + \frac{1}{2}K_{jk}(\Delta\nu_{jk})^2\} +$$

$$\sum_{i,j,k}\{H'_{ijk}r_{ij}r_{jk}(\Delta\Phi_{ijk}) + \frac{1}{2}H_{ijk}r_{ij}r_{jk}(\Delta\Phi_{ijk})^2\} +$$

$$\sum_{i,k}\{F'_{ik}q_{ik}(\Delta q_{ik}) + \frac{1}{2}F_{ik}q_{ik}(\Delta q_{ik})^2\} +$$

$$\sum_{j}K\omega_j(\Delta\omega_j)^2 + \sum_{j}K\tau_j(\Delta\tau_j)^2 \qquad (3)$$

, $\Delta\Phi_{ijk}$, $\Delta\omega_j$, $\Delta\tau_j$ are the internal coordinates corresponding to bond stretch, angle bend, out of plane deformation and torsion respectively and q represents non bonded nearest neighbor interactions. The potential energy distribution (PED) in the J^{th}

internal co-ordinate for the i[th] normal mode is given by

$$(PED)^{i}_{j} = \frac{L^{*}_{ji} L_{ji} F_{ji}}{\lambda_i} \qquad (4)$$

The estimate of the force constants for the force field was taken from the literature[36-37] and subsequently refined to match the observed spectra.

3. RESULT AND DISCUSSION

The FTIR spectra of title compound in KBr and dilute $CHCI_3$ solution are shown in Fig. 1-3. The-conformer structure diagram of the molecule is shown in figure. This is in line with the figure obtained from the X-ray diffraction[16]. The important calculated normal mode frequencies along with the observed frequencies in the FTIR spectra dilute $CHCI_3$ solution; their assignments are based on the concept of group frequencies and bond intensities. The internal co-ordinate and corresponding force constants are given in Table 3.

The NH mode of vibrations along with amide I and II band positions and their intensities are used with reasonable certainty to characterize the cis or tarns configuration and hydrogen binding effects in the secondary amide group. The strongest and most characterized bands of the secondary amides i.e amide I and amide II lie between 1500 and 1700 cm^{-1}[1,38]. The amide I band occurs at 1682 cm^{-1} in solution and solid phases both. This may again suggest to the existence of the intra-molecular hydrogen bonding. In the solid phase as it effects the resonance between C=O and C-N stretching causing decrease in the frequency.

The strong band at 1529 cm^{-1} in the solution phase is assigned to the amide II vibration. X-ray data shows that C-N bond lengths are shorter than the usual single C-N bond length. This is because of bond order sharing between C=O and C-N bonds in fact both bonds are equal bond orders, this may be ascribed to the increased bond order of the C-N bonds due to resonance stiffing. These increased bond order also contribute to the decrease in the frequency of N-H bending and a subsequent increase in corresponding force constant which is caused by the increased effective mass of the hydrogen due to the effect of the hydrogen bonding. The bond at 1503 cm^{-1} was assigned to semicircle stretching of pheny1-2 ring and the ring vibrations of pyrido, both were occurring at the same position. The bond is stable at 1503 cm^{-1} for pyrido as the environment around it is unchanged. However in the pheny1-2 ring due to substitutions of fluorine at meta position, the band is displaced to the lower side at 1470 cm^{-1} and is increased in intensity due to the enhancement of resultant dipole moment of phenyl ring. In fact it has become more intense than the 1503 cm^{-1} bond. The strong band at 1113 cm^{-1} and 1073 cm^{-1} assigned to the asymmetrical and symmetrical C-N stretching vibrations in the hetero-cycle piprazine ring system. This is same region in which C-N vibrations in the non cyclic tertiary amines have their absorption bands. The C-C and C-N band stretches couple with each other in this favorable environment.

The strong absorption bond at 1454 cm^{-1} is assigned to the CH_3 deformation frequency. This band shows the absence of ring strain in the chair conformation of the piprazine ring. The band at 1312 cm^{-1} is assigned to the CH_2 wagging vibrations. These bands are useful in the detection of the ring strain, as any non staggered chair conformation is evident from the X-ray data. The small lowering of the frequency of the band from aliphatic CH_2 wagging frequency at 1340 cm^{-1} is attributed to the presence of an N atom in the hetro-cyclic ring. The band at 1503 cm^{-1} was assigned to semicircle stretching of phenyl ring and the ring vibration of pyrido was occurring at the same position. The band is stable at 1503 cm^{-1} for pyrido as the environment around it is unchanged. However

in the Phenyl ring, due to substitution of fluorine at para position, the band is displaced to the lower side at 1470cm-1 and is increased in intensity due to enhancement of resultant dipole moment of phenyl ring. In fact, it has become more intense than the 1503 cm^{-1} band.

In case of tertiary amines the C-H stretching frequency of CH_3 group next to nitrogen atom become lower in frequency in addition to being intensified. Since the structure of the type CH_2-N-CH_2 is present in the component under study the band is displaced to a lower frequency and is highly intensified. Presence of a number of CH_2 group is a also factor in enhancing the intensity of the band. It has been shown for saturated hetro-cyclic rings containing one or two nitrogen, that they have as many skeletal stretching vibrations as they are skeletal bands if the two extreme frequencies, one involves the totally symmetric or ring breathing vibrations and is usually a strong Raman band and other involves, among other things, C-N-C asymmetric stretching which is usually a strong infrared band.

The medium intensity band at 1278 cm^{-1} is assigned to amide III and has major contribution form C-C stretching with lesser contribution of C-N stretch and C-C-C in plane bending.

The Strong absorption band at 610^{-1} is assigned as carbonyl vibration band. It seems that inductive effects play in tune of shift the frequency to higher side and to increase the intensity of the band.

The band at 1596 cm^{-1} is assigned to quadrant stretching of benzene rings. The out of plane bending variations of the hydrogen atoms in the two phenyl rings are complicated by the heavy substitutions viz. Pyrazino pyrido indole and carbonyl group. The situation becomes more so due to the presence of the piprazine ring vibrations in the same region.

Symmetric ring vibrations are assigned at 841 cm^{-1} although in the unstructured piprazine ring is asymmetrically substituted and gives a weak band in the infrared region. The strong absorption band at 610 cm^{-1} is assigned as wag mode of the carbonyl group. It seems that inductive effects, the frequency to higher side and to increase the intensity of the band. A strong band at 752 cm^{-1} and a medium band at 828 cm^{-1} are assigned to out of plane vibration of two adjacent hydrogen atoms. This is also evident form X-ray data.

The band at 1596 cm^{-1} is assigned to quadrant stretching of benzene rings. The out of plane bending variations of the hydrogen atoms in the two phenyl rings are complicated by the heavy substitutions viz. pyrazino pyrido indole and carbonyl group. The situation becomes more so due to the presence of the piprazine ring vibrations in the same region.

The band at 951 cm^{-1} is assigned to the symmetrical ring vibration of piprazine. The expected contribution of other C-C linkages in this absorption band is shown by the calculations. The interaction of the C-CH and N-C-H in plane bending due to the motion of the C atoms is also evident.

4. CONCLUSION

From the above study it is concluded that the large intensity is attributed to the presence of a large number of similar CH_2 groups and to Fermi resonance with the additive bending variation of CH_3 group. This variation along with ring breathing variations at 1113 and 1073 cm^{-1} have, previously also, been shown to confirm the presence of tertiary amines along with the presence of CH_2 group conjugated by a double bond in the molecule.

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Table 1 : X-ray data
a=8.434 (6) Å, b=6.620 (3) Å, c=18.419 (9) Å and â=95.07 (6)^0

No	Atom	x/a (σ)	y/b (σ)	z/c (σ)
1	C	4624(6)	5674(10)	7213(3)
2	C	3865(6)	3901(8)	7409(3)
3	C	3241(6)	3747(9)	8078(2)
4	C	3424(5)	5402(8)	8564(2)
5	C	4169(5)	7184(8)	8339(2)
6	C	4778(6)	7330(8)	3652(2)
7	C	2979(5)	5752(7)	9276(2)
8	C	3463(5)	7656(7)	9477(2)
9	N	4175(4)	8566(6)	8902(2)
10	C	2228(5)	4402(7)	9804(2)
11	C	1654(5)	5595(8)	10427(2)
12	N	2885(4)	7079(6)	10718(2)
13	C	3181(5)	8632(8)	10171(2)
14	C	1285(5)	4175(7)	11042(2)
15	N	705(4)	5220(7)	11653(2)
16	C	1926(5)	6659(8)	11946(3)
17	C	2317(6)	8119(7)	11352(2)
18	C	341(6)	3685(9)	12207(3)
19	C	-547(6)	4624(9)	12823(3)
20	C	-898(6)	2965(8)	13364(3)
21	C	-1847(7)	3730(10)	13961(3)
22	O	-2324(6)	5446(8)	13966(2)
23	C	-2247(6)	2331(10)	14561(3)
24	C	-1814(6)	314(10)	14556(3)
25	C	-2210(8)	-925(11)	15116(3)
26	C	-3003(8)	-135(11)	15656(3)
27	C	-3456(8)	1814(13)	15666(3)
28	C	-3081(8)	3053(11)	15107(3)
29	F	-3376(5)	-1376(8)	16211(2)

Table 2 : Cartesian Coordinates

No	Atom	X	Y	Z
1	C	2.725799507407430	3.7561880	13.2336433647987
2	C	2.053750833552830	2.5824620	13.5932432676825
3	C	1.418573644221860	2.4880514	14.8206531402806
4	C	1.493807837622680	3.5761240	15.7123141239618
5	C	2.158764747519300	3.5761240	15.2995081129983
6	C	2.784221030253240	4.8524600	14.0390737595231
7	C	1.002599980218120	3.8078240	17.0186158199885
8	C	1.378088.71315990	5.0682720	17.3873891817826
9	N	2.072183735090740	5.6706920	16.3324404870981
10	C	.2832620792214800	2.9141240	17.9873339177162
11	C	-.302257521007510	3.7038900	19.1303478947396
12	N	.6886007392386600	4.6862980	19.6642436689490
13	C	1.027284340081770	5.7143840	18.6606663889322
14	C	-.713577931827460	2.7638500	20.2586843247065
15	N	-1.30220464794289	3.4556400	21.3796817911451
16	C	-.320105935049980	4.4082580	21.9172471420887
17	C	.1063510285722400	5.3747780	20.8274392731451
18	C	-1.69937886451891	2.4394700	22.3961021148064
19	C	-2.55005161210016	3.0610800	23.5427854785939
20	C	-2.93268060780132	1.9628300	24.5188423578498
21	C	-3.83024309245093	2.4692600	25.6141543069396
22	O	-4.23335876083158	3.6052520	25.6233277738499
23	C	-4.26526729812893	1.5431220	26.7149703361756
24	C	-3.89926122974828	.20786800	26.7057968692653
25	C	-4.32440088838108	-.6123800	27.7332251632189
26	C	-5.08111487349128	-.0893700	28.7239595895313
27	C	-5.48604246374343	-.9109120	29.7422144165746
28	C	-5.46480281025258	1.2008680	28.7423065233519
29	F	5.087373252959100	2.0210860	27.7167129227804

Table -3 : Internet co-ordinates and their force constants

Internet co-ordinates	force constants ($x10^5$ dynes/cm)
v(C-C)	5.790
v(C-C)	3.720
v(C-C)	4.000
v(C-C)	4.200
v(C-N)	3.350
v(C-N)	3.830
v(C-N)	3.100
v(C-N)	3.900
v(C=O)	8.730
v(C-F)	6.250
ϕ (C-C-C)	0.500(0.400)
ϕ (C-C-C)	0.510(0.400)
ϕ (N-C-C)	0.410(0.220)
ϕ (N-C-C)	0.420(0.200)
ϕ (C-N-C)	0.410(0.150)
ϕ (C-C=O)	0.250(0.050)
ϕ (C-C-F)	0.950(0.750)
ω (C=O)	0.400
ω (C-F)	0.600
τ (C-C)	0.037
τ (C-C)	0.037 0.030
τ (C-N)	0.040

❖ The value in parenthesis represent non-bonded nearest neighbor interactions.

Table 4 : Normal mode frequencies and their assignments

Frequencies (in cm^{-1})			**Assignments** (PED is given in % with in square brackets and the group are given with in braces)
Calculated	Observed		
	$CHCl_3$	KBr	
1680	1682	1682	v(C-C) [39] +v (C=O) [56] {carbonyl}
1647	1655	1653	v(C-C) [87] + ϕ(C-C-C) [13] {pyrido-phenyl-1}
1586	1596	1597	v(C-C) [89] + ϕ (C-C-C) [10]
1577	1576	1575	v(C-C) [85] {carbonyl}
1529	1529	1526	v(C-C) [95] {phenyl-2}
1504	1503	1501	v(C-C) [72] + v(C-C) [11] {pyrido}
1473	1470	1471	v(C-C) [25] + v(C-C) [20] + v(C-F) [38] {phenyl-2-F}
1472	1470	1471	v(C-C) [92] {phenyl-1}
1436	1435	1430	v(C-C) [82] + ϕ(C-C-C) [10] {phenyl-1}
1389	1388	1385	v(C-C) [12] + v(C-C) [73] + ϕ(C-C-F) [11] {phenyl-1}
1353	1361	1360	v(C-C) [51] + v(C-F) [31] {phenyl-2-F}
1328	1332	1336	v(C-C) [82] {piprazine}
1309	1312	1310	v(C-C) [83] {CH_2 Wagging}
1270	1278	1275	v(C-C) [53] + v(C-C) [21] + v(C-N) [16] +ϕ(C-C-C) [10] {phenyl-1}
1252	1258	1260	v(C-C) [41] + v(C-c) [11] + ϕ (C-C-F) [18] {phenyl-2}
1245	1238	1240	v(C-C) [50] + v(C-C) [14] + v(C-N) [22] + ϕ(C-C-C)[11] {phenyl-1}
1206	1201	1205	v(C-C) [75] + v(C-N) [10] {CH_2 Wagging}
1183	1182	1185	v(C-C) [41] + v(C-N) [45] {pyridine}
1146	1151	1152	v(C-C) [48] +v(C-N) [20] {phenyl-1}
1112	1111	1112	v(C-C) [22] +v(C-N) [56] {piprazine}
1097	1098	1097	v(C-C) [67] {phenyl-2}
1069	1073	1070	v(C-C) [17]+v(C-N) [19]+v(C-N)[12]+v(C-N)[30] {piprazine ring vibrations}
1050	1056	1059	v(C-C) [59] + v(C-N) [17] {phenyl-1}
1033	1035	1035	v(C-C) [17] + v(C-N) [20] +v(C-N) [18]+ϕ(C-C-C) [15] {pyridine}
1010	1009	1010	v(C-C) [23] +v(C-N) [21] +v(C-N)[10]+ϕ(C-C-C) [15] {pyridine}
955	989	990	v(C-C) [31] +v(C-N)[10] + v(C-N) [21] {piprazine}
956	951	955	v(C-C) [25] +v(C-N) [43] {piprazine}

Table 4 : (Contd.....)

Frequencies (in cm^{-1})			**Assignments** (PED is given in % with in square brackets and the group are given with in braces)
Calculated	Observed		
	$CHCl_3$	KBr	
936	932	935	v(C-C) [29] +v(C-C) [27] +ϕ(C-C-C) [13] {phenyl-1}
898	900	905	v(C-C) [21]+v(C-C)[18]+v(C-N)[13]+v(C-N)[11]+ϕ(C-C-C)[19]{piprazine pyrido indole}
843	841	840	v(C-N) [43] +v(C-N) [16] {piprazine}
796	792	795	v(C-C) [29] +v(C-C) [35] {phenyl-2}
785	792	795	ω(C-F) [88] {carbonyl}
779	778	780	v(C-N) [15] +v(C-N) [52] {piprazine}
708	708	710	v(C-C) [15] +v(C-N) [24] +ϕ(C-C-C) [45] {pyrido}
705	708	710	v(C-C) [14] +ϕ(C-C-C) [11] +ϕ(C-C-C) [10] {phenyl-2-F}
683	689	690	v(C-C) [22]+v(C-C) [13]+v(C-N) [14]+ϕ(C-C-C) [27] {pyridine}
608	610	605	ω(C=O) [91] {carbonyl}
598	599	595	ϕ(C-C-C) [55] +ϕ(N-C-C) [14] {indole}
559	559	560	v(C-C) [11] +ϕ(C-C-F) [46] {phenyl-2-F}
542	542	547	ϕ(C-C-C) [43] +ϕ(N-C-C) [19] +ϕ(C-N-C) [17] {pyrido}
504	502	502	ϕ(C-C-C) [26] {aliphatic}
493	495	492	ϕ(C-C-C) [19] +ϕ(C-C-C) [15] {phenyl-2}
482	489	482	ϕ(C-C-C) [23] +ϕ(C-C-C) [11] {phenyl-2}
477	468	472	ϕ(C-C-C) [52] +ϕ(N-C-C) [18] {pyrido}
452	448	457	ϕ(C-C-C) [46] +ϕ(N-C-C) [16] +ϕ(N-C-C) [11] +ϕ(C-N-C) [11] {pyridine}
412	414	415	ϕ(C-C-C) [29] +ϕ(N-C-C) [14] +ϕ(N-C-C) [15] +ϕ(C-N-C) [15] {piprazine}
402	401	399	ϕ(C-C-C) [27] +ϕ(N-C-C) [21] +ϕ(C-N-C) [12] {piprazine}
385	388	386	ϕ(C-C-C) [21] +ϕ(N-C-C) [10] +ϕ(C-N-C) [29] {piprazine}
363			ϕ(N-C-C) [32] +ϕ(N-C-C) [11] +ϕ(C-N-C) [33] {piprazine}
348			ϕ(C-N-C) [21] {piprazine}
326			ϕ(C-C-C) [13] +ϕ(N-C-C) [11] +ϕ(C-N-C) [46] {piprazine}
315			τ(C-C) [85] {phenyl-1} ϕ(N-C-C) [35] +ϕ(C-N-C) [20] +τ(C-C)[24] {piprazine} ϕ(C-C-C) [33] + ϕ(C-N-C) [14] {aliphatic}
266			τ(C-C) [37] +τ(C-N) [37] {pyrido}
255			ϕ(C-C-C) [31] +ϕ(C-N-C) [17] {aliphatic}

Table 4 : (Contd.....)

Frequencies (in cm^{-1})			**Assignments** (PED is given in % with in square brackets and the group are given with in braces)
Calculated	Observed		
	$CHCl_3$	KBr	
229			ϕ(N-C-C)[12] +ϕ(C-N-C)[13] +τ(C-C)[48] {phenyl-1}ϕ(C-C-C)[16] +ϕ(C-N-C) [15] +ϕ(C-C-O) [22] {corbonyl}
			ϕ(N-C-C) [11] +ϕ(C-N-C) [14] +τ(C-C) [47] +τ(C-N) [13] {phenyl-1} ϕ(C-C-C) [12] +ϕ(C-C-O) [30] +τ(C-C) [18] {corbonyl}
172			ϕ(C-N-C) [11] +τ(C-C) [45] {phenyl-1} ϕ(C-C-C) [11] +ϕ(N-C-C) [15] +ϕ(N-C-C) [14] +τ(C-C) [31] +τ(C-N) [12] {pyridine}
148			τ(C-C) [73] {pyridine}
139			ϕ(C-C-C) [25] +ϕ(C-N-C) [30] {piprazine}
132			τ(C-C) [15] +τ(C-C) [44] {corbonyl}
113			ϕ(N-C-C) [17] +ϕ(C-N-C) [18] +τ(C-C) [20] +τ(C-N) [19] {pyridine}
100			τ(C-C0 [62] +τ(C-N) [13] {phenyl-1}
91			ϕ(C-C-C) [26] +ϕ(N-C-C) [17] {corbonyl} τ(C-C) [49] {corbolyl}
66			τ(C-C) [15] {phenyl-2}
62			ϕ(C-C-C) [12] +τ(C-C) [29] [corbonyl}
56			τ(C-C) [29] +τ(C-C) [43] {corbonyl}
49			ϕ(C-N-C) [15] +τ(C-C) [29] +τ(C-N) [12] [corbonyl}
30			τ(C-C) [58] +τ(C-N) [14] {corbonyl} ϕ(C-C-C) [12] +ϕ(N-C-C) [12] +ϕ(C-N-C) [11] + τ(C-C) [39] {pyrido}
21			τ(C-C) [52] + τ(C-N) [22] {indole}
14			τ(C-C) [13] {phenyl-2} ϕ(N-C-C) [16]+τ(C-C) [11] +τ(C-C) [11] +τ(C-N) [12] {piprazine}
			τ(C-C) [72] {aliphatic} ϕ(N-C-C) [16] +τ(C-C) [14] +τ(C-C) [29] +τ(C-N) [27] {corbonyl} τ(C-C) [48] +τ(C-N) [23] {phenyl-1}
4			τ(C-C) [25] {phenyl-2}

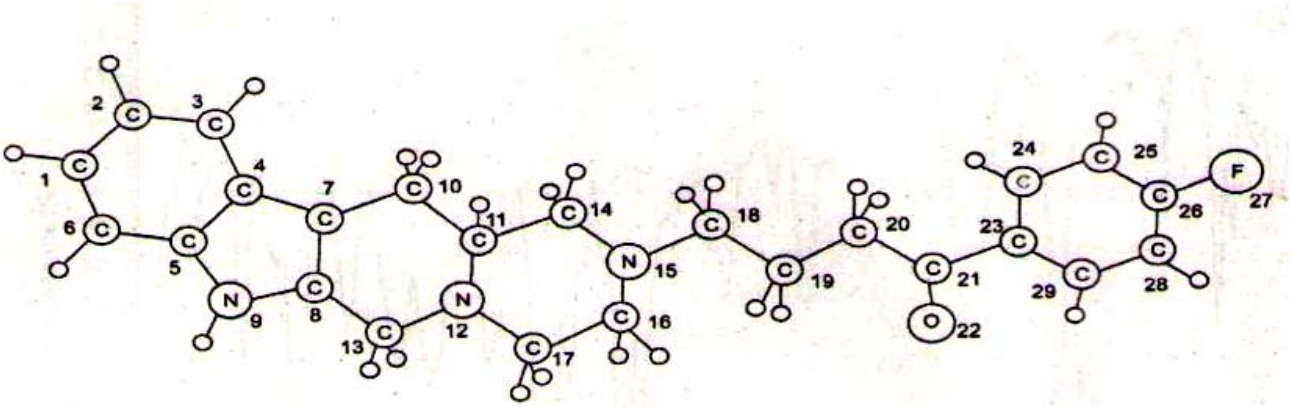
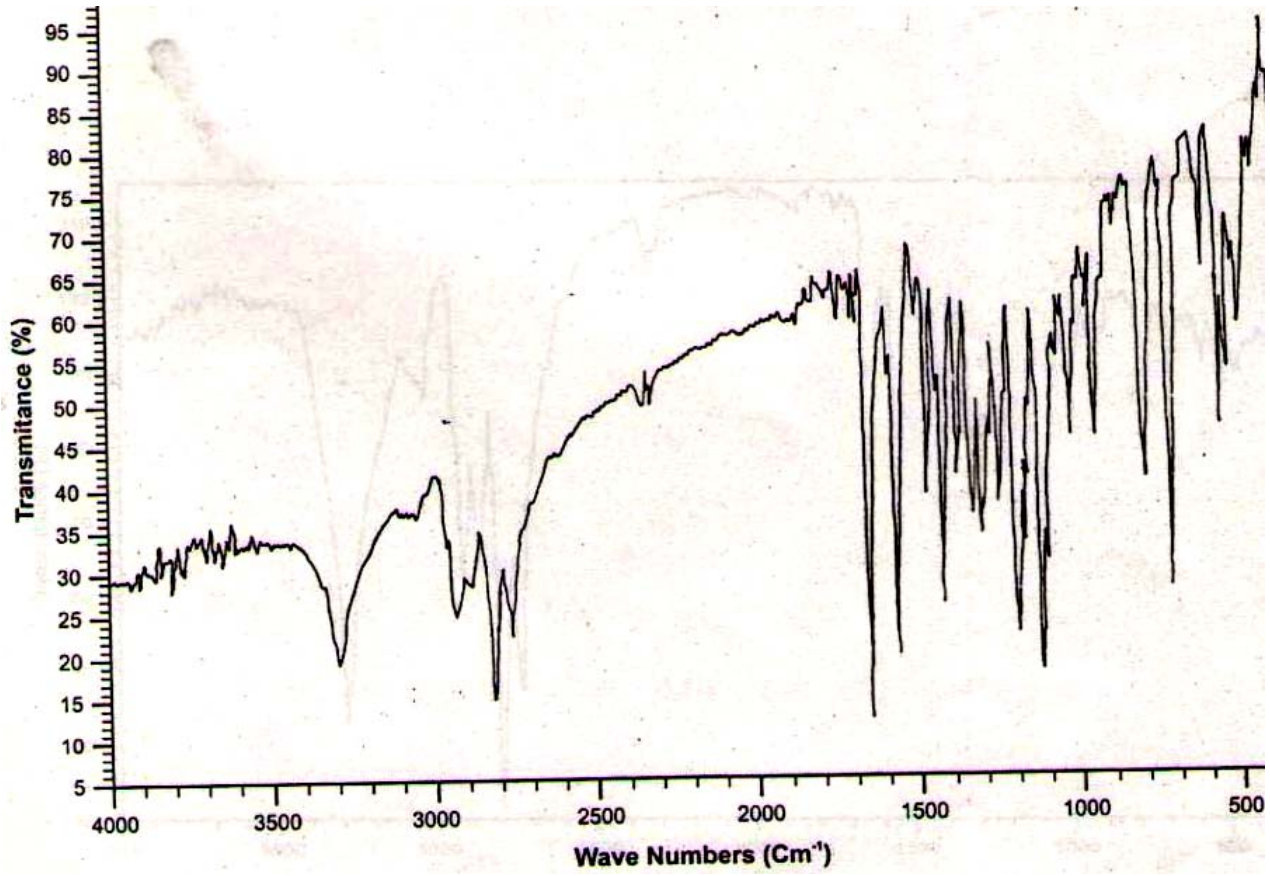
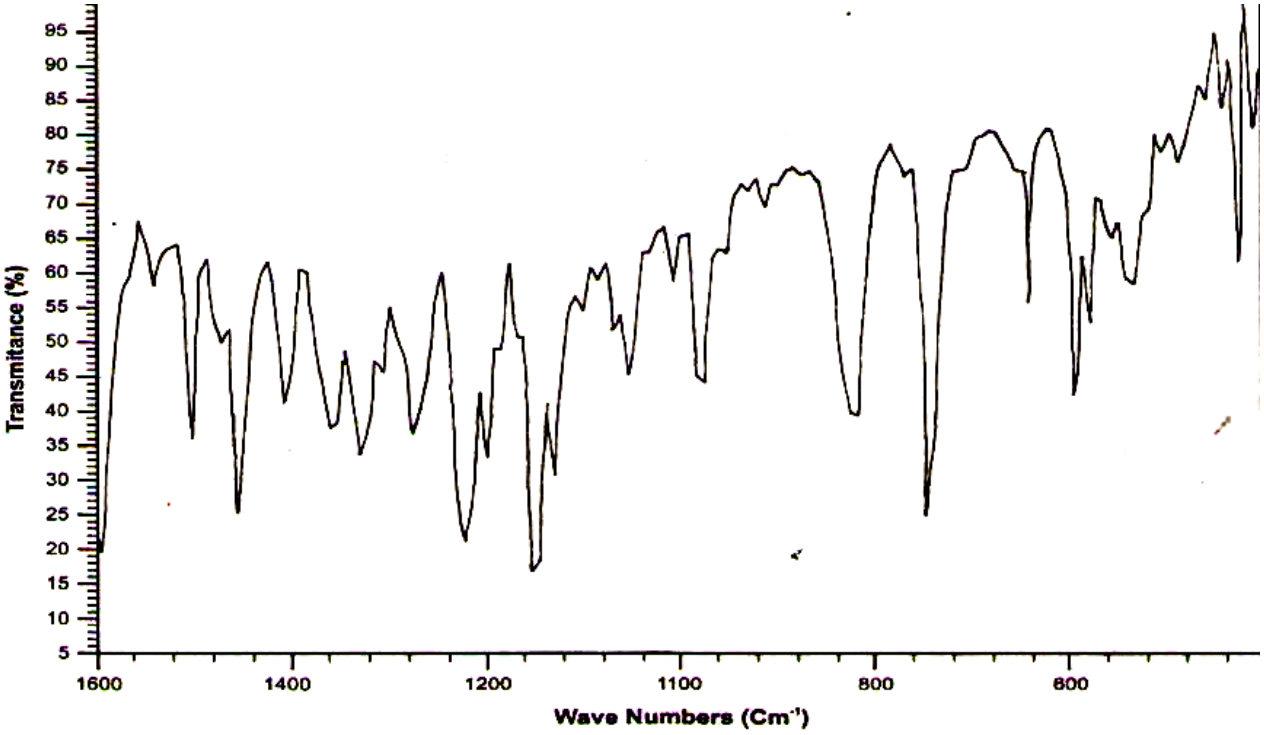


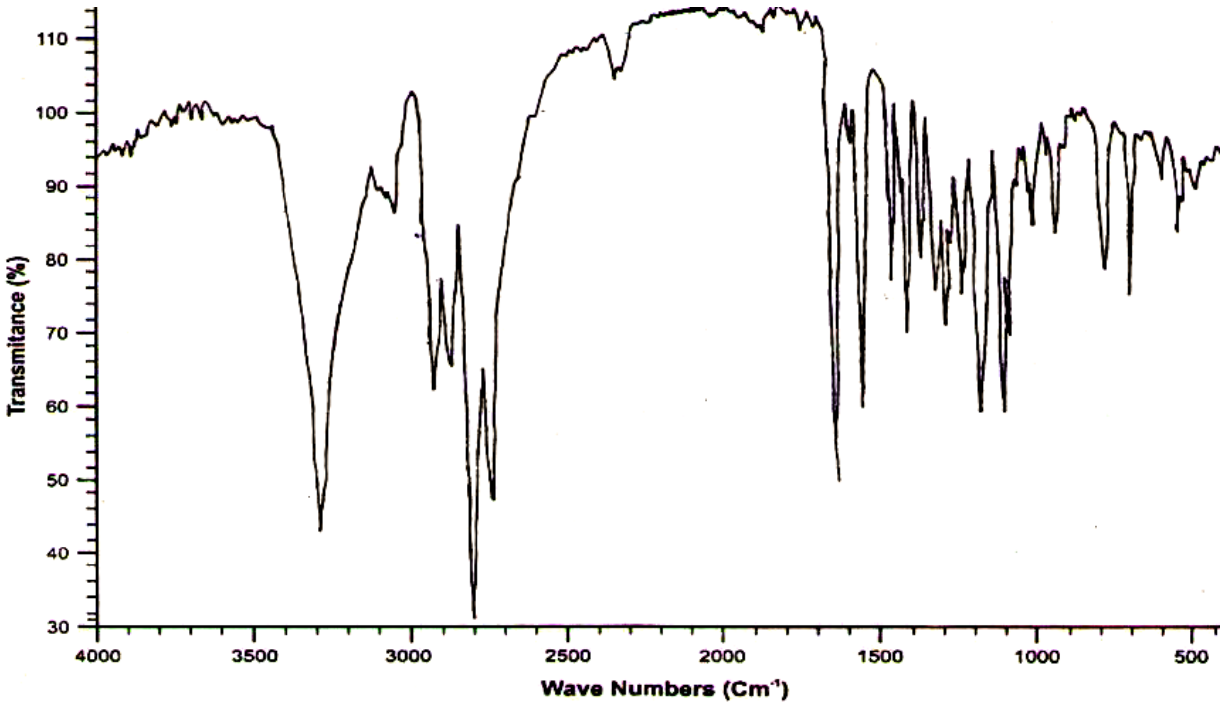
Fig. 1: 2[3(p-flourobenzoyl) propyl]-1,2,3,4,6,7,12,12a-octahydropyrazino [2',1':6,1] pyrido [3,4-b] indole[centbutindole]



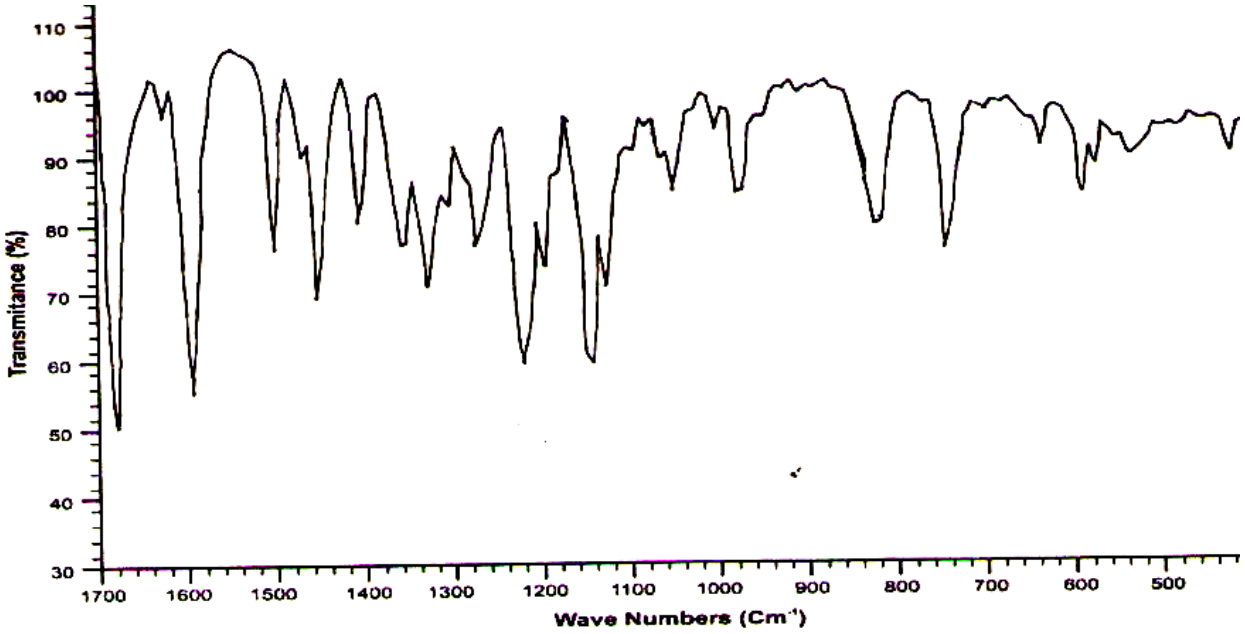
(a)



(b)



(c)



(d)

Fig. 2: Transmittance percentage versus Wave numbers (Cm^{-1}) ranging from (a) 500-4000, (b)500-1600, (c)500-4000 and (d)500-1700

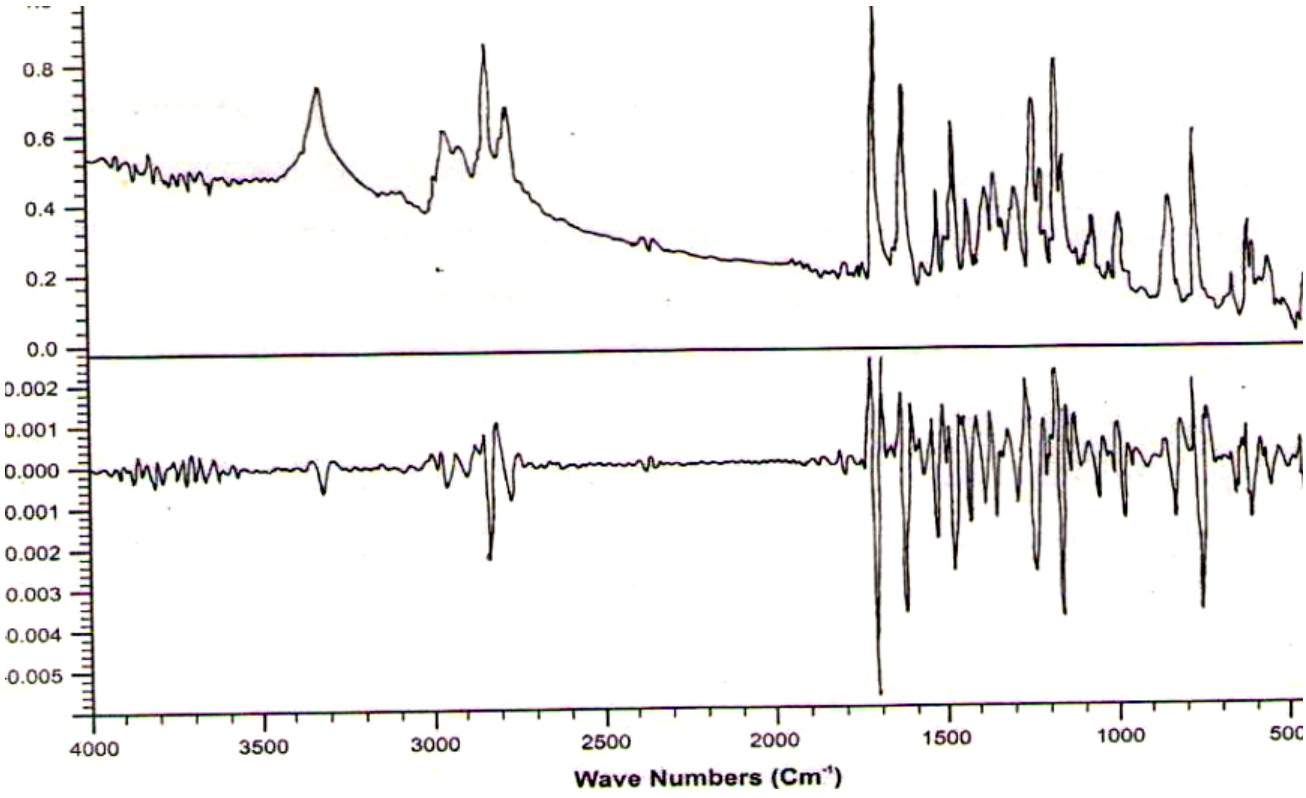


Fig. 3: Simulation versus Wave numbers (Cm^{-1})

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