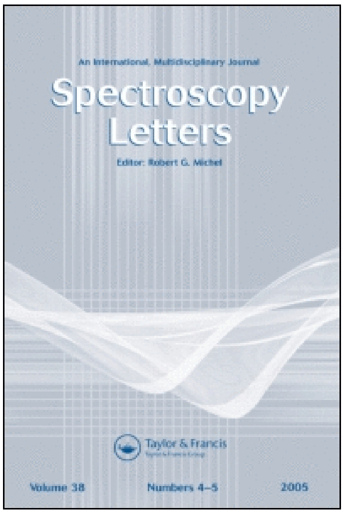

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Vibrational Spectra and Conformational Analysis of Isomers of 1,3-Diphenyl Propane and 4-(3-Phenyl Propyl)Pyridine

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VIBRATIONAL SPECTRA AND CONFORMATIONAL ANALYSIS OF ISOMERS OF 1,3-DIPHENYL PROPANE AND 4-(3-PHENYL PROPYL)PYRIDINE

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ABSTRACT

The Raman and infrared spectra of 1,3-diphenyl propane and 4-(3-phenyl propyl)pyridine were recorded in the liquid state, at room temperature, in the range from 4000 cm^{-1} to 200 cm^{-1}. The vibrational assignments allowed us to identify the presence of three staggered conformers, AA, AG and GG. No evidence was found of existence of the GG_1 conformer with the two parallel phenyl (or pyridil) ring groups. These results have been used to correlate the normal modes from these molecules with those from the polystyrene and polyvinylpyridine.

I. INTRODUCTION

The vibrational spectra and molecular structure of polystyrene has been reported by many persons(1-5) and many difficulties found to assign the nor-

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mal modes. Recently Jasse and col.(6-9) had reported studies related with molecular models for this polymer and were able to show the influence of the chain conformations and configurations on the infrared and Raman spectra of these models. These studies were very helpful in the identification of the conformational sequencies of the aliphatic chain with alternated phenyl groups as substituents and the chain termined with methyl groups. Others persons had studied molecular models for polystyrene which were n-alkylbenzene derivatives and also in these cases the models have methyl groups in the end of the aliphatic chain. Although the importance of these studies, the presence of the methyl groups added additional complications in the assignment of their normal modes due to the interactions between this group and many other normal modes by the ring, making impossible an undought assignment of the vibrational spectra. No complete study was done in the case of the polyvinylpyridine molecule.

We have chosen the 1,3-disubstituted propanes, as 1,3-diphenyl propane (DFP) and 4-(3-phenyl propyl)pyridine (FPPy), to resolve partially the problem of the assignments of the vibrational frequencies, since they don't have methyl-groups in the aliphatic chain. However the spectra remained still complicated because of the number of the normal modes and the interactions between the aliphatic and ring groups the molecules. By comparing the DFP and FPPy spectra (wave numbers and contour of the bands) it was possible to separate the wave numbers of the normal modes from the rings and from the aliphatic chain, as well to identify the presence of three stable conformers in the liquid state, at room temperature. These conformers are specified by the notation AA, AG and GG, where A and G notation describe anti and gauche configurations between a C-ring and a next to nearest C-C bond,(12) as shown in the figure 1.

The comparison between the wave numbers of the normal modes from the DFP with those from polystyrene and from the FPPy with those from polyvinyl-

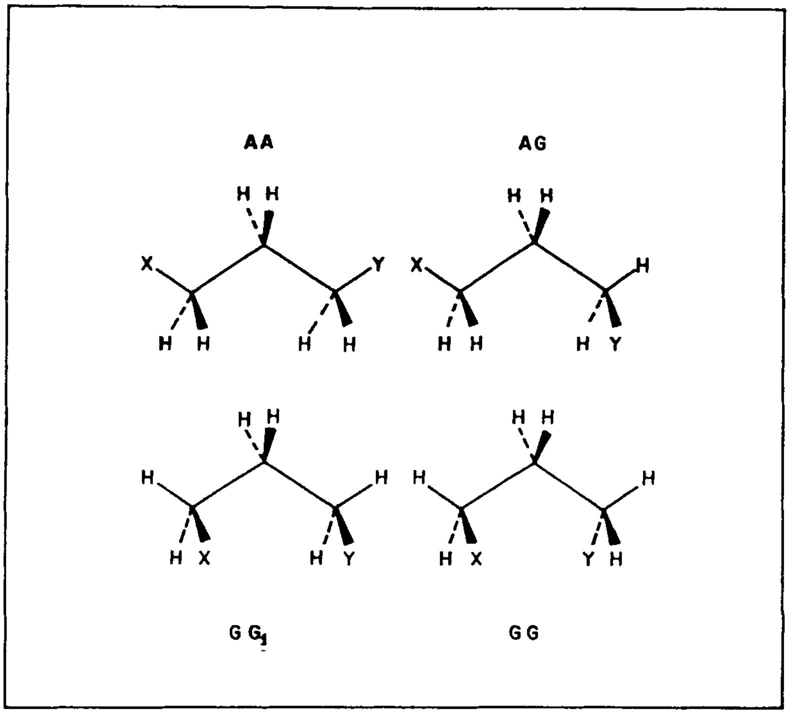

FIGURE 1. The staggered conformers of 1,3-disubstituted propanes: X=Y=phenyl groups in the case of DFP; X = phenyl group, Y = pyridil group, in the case of FPPy.

pyridine have indicated that the conformations of the polymer chains are the same in both cases.

II. MATERIALS AND METHODS

The Raman spectra were recorded employing an argon ion laser (Spectra Physics model 165) using the 514.5 nm laser line as excitation. A Spex 1401B double monocromator equipped with a 1800 g/mm holographic gratting was employed as a spectrometer and a termoelectricaly cooled RCA C3103 photomulti-

TABLE 1. Comparison of the symmetry species and wavelengths of the normal modes of benzene and pyridine rings in the DFP and FPPy molecules - conformational independent normal modes.

Vibration number	Symmetry species in benzene	Symmetry species in DFP and FPPy	$\bar{\nu}_{predict}$ range(10)	$\bar{\nu}_{observed}$ benzene ring (cm^{-1})	$\bar{\nu}_{observed}$ pyridine ring (cm^{-1})	$\bar{\nu}_{polystyrene}$(1) (cm^{-1})
ν_1 ϕ_{CCC}	A_{1g}	A'	620-830	796	791	797
ν_2 ν_{CH}	A_{1g}	A'	3030-3070	3054	3050	3050
ν_3 β_{CH}	A_{2g}	A'	1270-1331	1329	1294	1306
ν_4 γ_{CC}	B_{2g}	A"	680-700	699	715	705
ν_5 γ_{CH}	B_{2g}	A"	970-1000	980	872	987
ν_{6a} ϕ_{CCC}	E_{2g}	A'	300-530	494-486	498-502	444
ν_{7a} ν_{CH}	E_{2g}	A'	3000-3060	3037	-	3033
ν_{8a} ν_{CC}	E_{2g}	A'	1575-1614	1601	1598	1602
ν_{9a} β_{CH}	E_{2g}	A'	1170-1181	1175	1217	1183
ν_{6b} ϕ_{CCC}	E_{2g}	A'	605-630	619	667	622
ν_{7b} ν_{CH}	E_{2g}	A'	3030-3080	3061	3043	3060
ν_{8b} ν_{CC}	E_{2g}	A'	1562-1597	1580	1558	1583

Table 1. Continuation

ν_{10a}	γ_{CH}	E_{1u}	A"	810-860	840	814	844
ν_{11}	γ_{CH}	E_{1u}	A"	720-830	743	835	762
ν_{12}	β_{CCC}	B_{1u}	A'	990-1010	1002	990	1002
ν_{13}	ν^{s}_{CX}	B_{1u}	A'	1100-1280	1120	1120	-
ν_{13}	ν^{a}_{CX}	B_{1u}	A'	1100-1280	1204	1210	1200
ν_{14}	ν_{CC}	B_{2u}	A'	1300-1350	1379	1379	1327
ν_{15}	β_{CH}	B_{2u}	A'	1150-1160	1155	-	1156
ν_{16a}	γ_{CC}	E_{2u}	A"	390-420	396	405	407
ν_{17a}	γ_{CH}	E_{2u}	A"	940-980	968	976	967
ν_{17b}	γ_{CH}	E_{2u}	A"	830-940	903	-	907
ν_{18a}	β_{CH}	E_{1u}	A'	1018-1030	1028	1068	1031
ν_{19a}	β_{CH}	E_{1u}	A'	1470-1515	1495	1495	1495
ν_{20a}	ν_{CH}	E_{1u}	A'	3070-3110	3084	3070	3081
ν_{18b}	β_{CH}	E_{1u}	A'	1065-1082	1082	1115	1074
ν_{19b}	ν_{CC}	E_{1u}	A'	1440-1470	1450	1411	1450
ν_{20b}	ν_{CH}	E_{1u}	A'	3020-3080	3025	3030	3025

ν = stretching, a = antisymmetric, s = symmetric, ϕ = in-plane ring deformation,
β = in-plane bending, γ = out-of-plane deformation, X = substituent.

plier tube detector was coupled with a photon counting system. The spectral slit width was 3 cm^{-1} and the resolution was $< \pm 1$ cm^{-1}.

Infrared spectra of liquid samples were recorded on a Perkin Elmer model 180 spectrophotometer using a CsI selead liquid cell with path length of 0.05 mm.

1,3-diphenyl propane (Frinton Lab.) and 4-(3-phenyl propyl)pyridine (ICN Pharmaceuticals Inc.) were chromatographed over dry Al_2O_3 and silica gel. The solvent was evaporated and the sample was dried in a vacuum immediately before the use. An uncorless liquid was obtained in both cases.

III. RESULTS

The normal modes of the phenyl group has been assigned upon analogy with the vibrations of monosubstituted benzenes as used by Varsanyi(10). It is assumed that the molecules belong to the Cs point group, with the C_α-H bonding coplanar with the benzene ring.(7) In this situation all of the normal models must be active either in the case of the Raman or infrared spectra.

The normal modes from the benzene or pyridine ring, can be divided in three classes: 1. the mass insensitive normal modes, which have stable wave numbers independent on the alkyl group; 2. the mass sensitive normal modes, whose wave numbers change by the effect of the substituent(10); 3. the conformational sensitive normal modes, whose wave numbers are dependent on the conformation of the aliphatic chain(6-9). The identification of these normal modes are shown in the table 1, in the case of the classes 1 and 2, and in the table 2, in the case of the class 3. The normal modes of the class 3 were identified as: in-plane bending from the bonding ring-substituent, and the out-of-plane angle deformations from the ring and from the ring-substituent groups(6-9).

TABLE 2. Symmetry species and wavelengths of the normal modes of benzene and pyridine rings - conformational dependent modes.

Vibration number	Symmetry species in benzene	Symmetry species in DFP and FPPy	Predict $\bar{\nu}$ range (cm^{-1})	$\bar{\nu}_{observed}$ benzene	$\bar{\nu}_{observed}$ pyridine	Conformer	$\bar{\nu}_{observed}$ polystyrene(1)
ν_{9b} β_{CX}	E_{2g}	A'	200-410	230	228	AA	
				214	216	AG	
				206	204	GG	222
ν_{10b} γ_{CX}	E_{1g}	A"	140-200	150		AG	155
				162		AA, GG	
				181		AG	
ν_{16b} γ_{CC}	E_{2u}	A"	430-560	544	552	GG	542
				556	564	AG	
				570	578	AA	

β = in-plane bending, γ = out-of-plane deformation.

The 1,3-disubstituted propanes have nine possible conformations of the aliphatic chain, exclusive of several cis forms(11,12). The order of stability for these conformers are AA > AG = AG_1 ~ GA = G_1A > GG = G_1G_1 > GG_1 = G_1G. The equivalent GG_1 and G_1G forms are not possible due to large steric and electrostatic repulsions between the two rings(12). This conformer may be observed in the electronic excited state and it is known as the structure of the eximer from DFP(13). If the two substituents as identical, the two forms AG and GA are equienergetics and only three conformers may be observed in the liquid state, as indicated in the figure 1 and table 2.

3.1. Conformational Independent Normal Modes

Stretching CH normal modes

There are five normal modes for the CH stretching vibrations of monosubstituted benzene rings and four for pyridine ones. Three of them are identified in the infrared spectra, as a strong bands in crescent order of intensity, as ν_{20a}, ν_{7b} and ν_{20b}. The normal mode ν_2 is assigned as the most intense Raman band and the normal mode ν_{7a} could be assigned in the Raman spectra, since it is not resolved in the infrared(10) (figure 2). This normal mode is absent in the pyridine monosubstituted ring(14-19). The wavelengths of these normal modes are given, as for the others below in the table 1.

Stretching CC (CN) normal modes

The tangential stretching CC and CN vibrations from the rings are almost insensitive to substitution and they can be shared in two groups: 1. the normal modes ν_{8a} and ν_{19a}, with wave numbers independent on the nitrogen atom in the ring and, 2. the normal modes ν_{8b} and ν_{19b} whose wave numbers for the case of the pyridine group are shift 40 cm^{-1} from those of benzene ring(10).

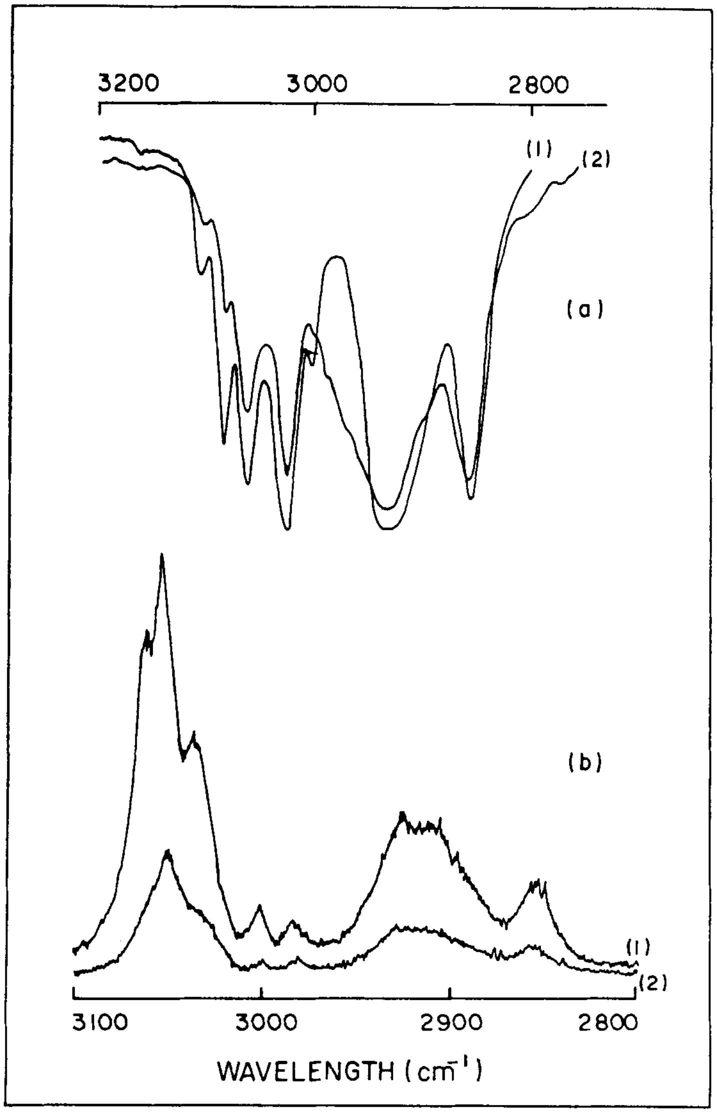

FIGURE 2. Infrared (a) and Raman (b) spectra of DFP (1) and FPPy (2) in the range of 3200-2800 cm^{-1}.

The normal mode ν_{14} was observed at 1379 cm^{-1} for the case of DFP and at 1379 cm^{-1} for the case of pyridine ring of FPPy, both as medium intensity bands in the infrared spectra, as shown in the figures 3 and 4.

Stretching C-X normal modes

The normal mode related to the C-X stretching vibration was identified by ν_{13} for light substituent(10). This normal mode can be considered as a combination of symmetric and antisymmetric motions of the ring-substituent vibrations, as was done by Pearce(20). In this sense, we have assigned the wavelength at 1204 cm^{-1} for the antisymmetric C-X stretching of DFP (1210 cm^{-1} for FPPy) and the wave number at 1120 cm^{-1} to the symmetric C-X stretching. This last band is intense in the Raman spectra and its wave number and intensity don't change in the case of DFP or FPPy, as shown in the figure 4.

In-plane C-H bending deformations

The in-plane C-H bending deformations of monosubstituted benzenes are identified as ν_3, ν_{9a}, ν_{15} (absent for monosubstituted pyridines)(17), ν_{18a} and ν_{18b}(10). The assignment of the wave number for the normal mode ν_{15} was done as used for n-alkylbenzenes(10) in the case of the DFP, as shown in the figure 4. In the case of FPPy, we could notice that the intensity of the band at 1155 cm^{-1}, in the infrared spectra, had lower intensity than in the case of the DFP and no new band could be observed, which indicates that this normal mode is absent in the pyridine ring, diferently from what is assigned by other persons(16,18,19).

In-plane ring bendings

These deformations are identified by ν_1 (ring breathing), ν_{6a}, ν_{6b} and ν_{12}(10). The normal modes ν_1 and ν_{6b} are almost insensitive to substitution

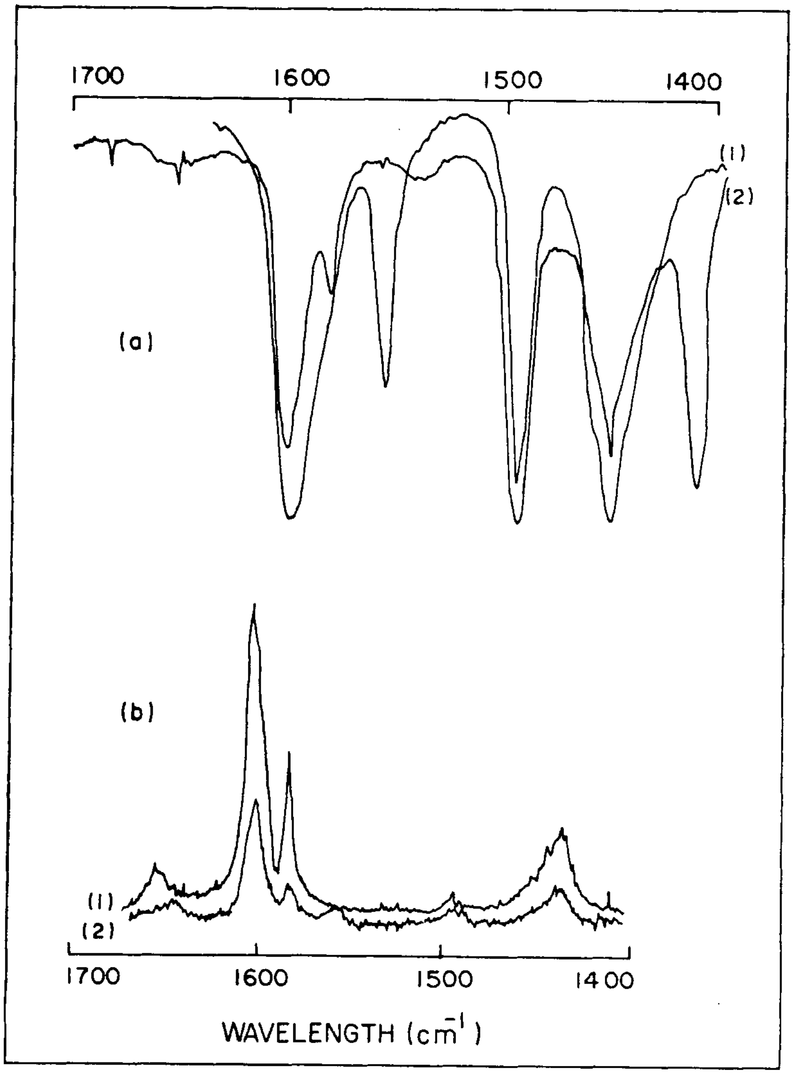

FIGURE 3. Infrared (a) and Raman (b) spectra of DFP (1) and FPPy (2) in the range of 1700-1400 cm^{-1}.

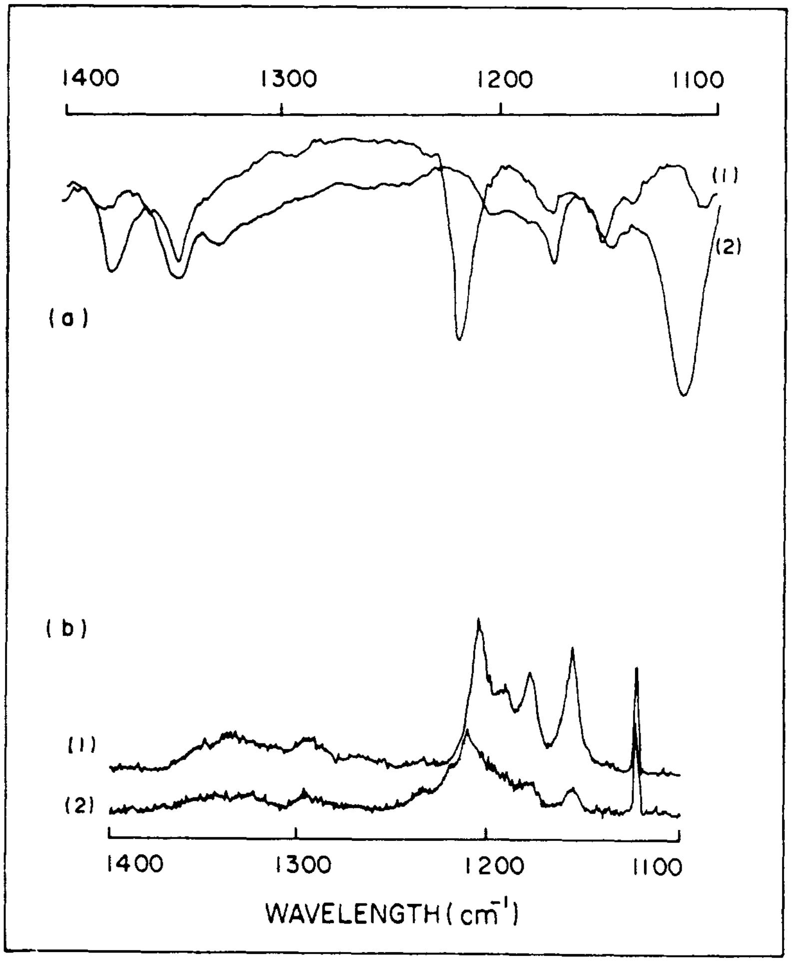

FIGURE 4. Infrared (a) and Raman (b) spectra of DFP (1) and FPPy (2) in the range of 1400-1100 cm^{-1}.

for monoalkylbenzenes or pyridines, while ν_{6a} is a substitution sensitive normal mode. The region of wave numbers in which these normal modes can be observed(1,10,15) and their wave numbers for DFP and FPPy are shown in the table 1, and their Raman and infrared spectra in the figures 5, 6 and 7.

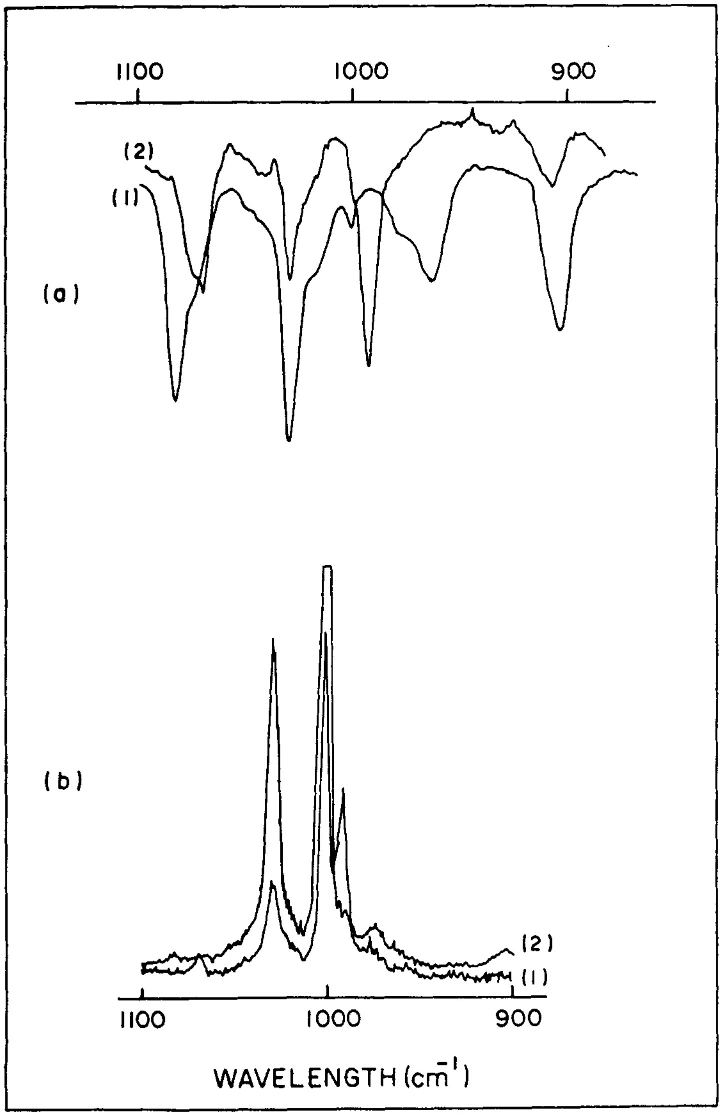

FIGURE 5. Infrared (a) and Raman (b) spectra of DFP (1) and FPPy (2) in the range of 1100-900 cm^{-1}.

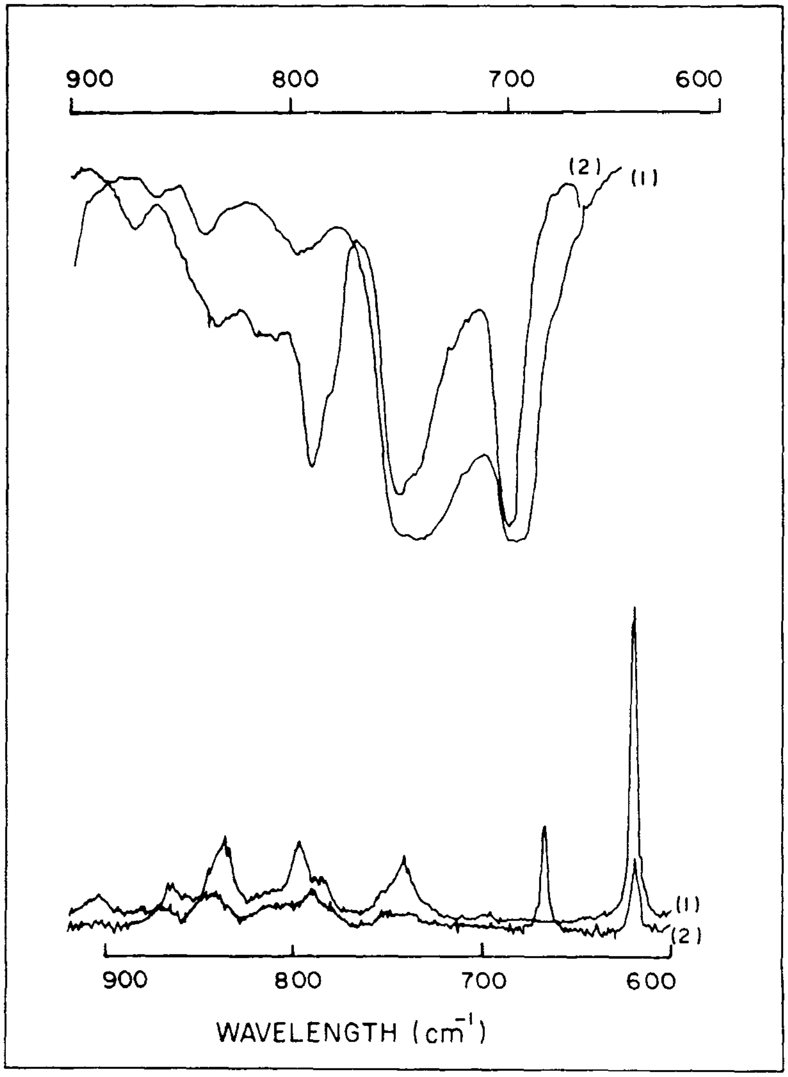

FIGURE 6. Infrared (a) and Raman (b) spectra of DFP (1) and FPPy (2) in the range of 900-600 cm^{-1}.

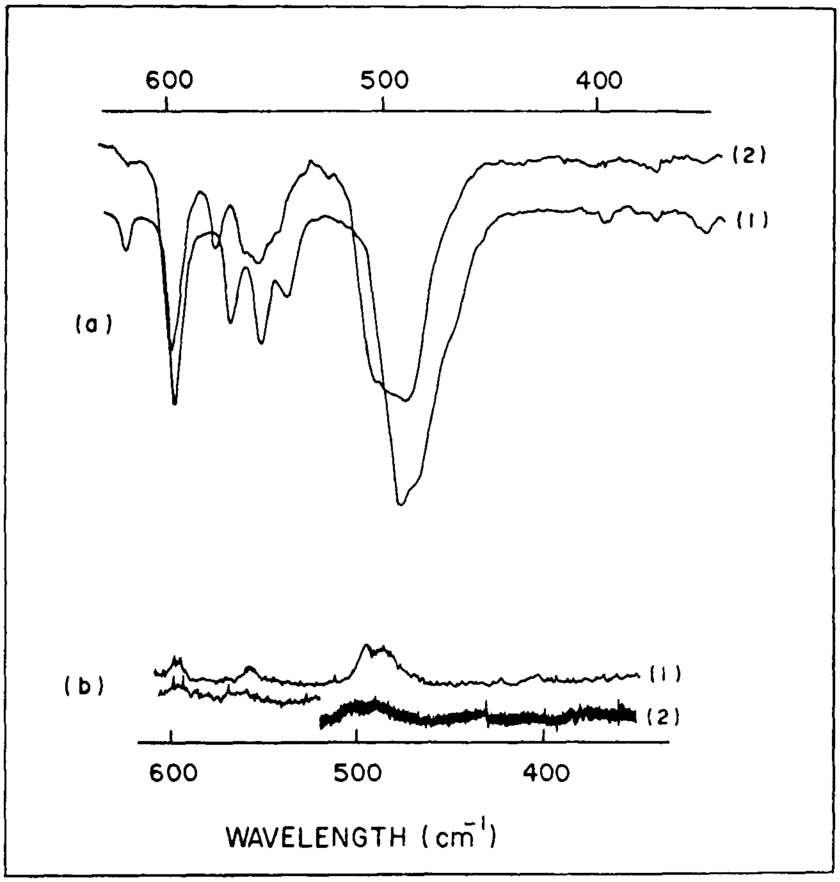

FIGURE 7. Infrared (a) and Raman (b) spectra of DFP (1) and FPPy (2) in the range of 600-400 cm^{-1}.

Out-of-plane γ_{CH} vibrations

These are five out-of-plane γ_{CH} vibrations for monosubstituted benzenes and four for pyridine ones, as shown in the table 1. These normal modes are identified as ν_5, ν_{10a}, ν_{11}, ν_{17a} and ν_{17b} (absent for pyridine ring)(10,14-19). These normal modes show high intensities bands in the infrared spectra, low intensity bands in the Raman spectra and overtones or combination bands in the range of 1650-2000 cm^{-1} (10). These observations have allowed us to assign the wave numbers to these normal modes, as shown in the table 1 and in the figures 5 and 6.

Out-of-plane ϕ_{CC} ring deformations

These normal modes are identified as ν_4, ν_{16a}, which are weak bands in the infrared spectra, insensitive on monosubstitution(10), and ν_{16b}, ν_a conformational dependent normal mode(6-9). The wave numbers of the ν_4 and ν_{16a} normal modes are given in the table 2 and figures 5 and 6 respectively, while ν_{6b} will be considered bellow.

3.2. Conformational Dependent Normal Modes

There are three normal modes of the benzene ring which wave numbers are clearly shifted by the influence of the conformation of the aliphatic chain(6-9). These normal modes are: the in-plane β_{CX} deformation, ν_{9b}; the out-of-plane γ_{C-X} deformation, ν_{10b}; and the out-of-plane ring deformation, ν_{16b}(10).

We have observed in the infrared spectrum of DFP three bands in the region of 560 cm^{-1}, as shown in the figure 7, which can be assigned to the normal mode ν_{16b} from distinct conformers(6-9). By comparing the bands from benzene ring with those from the pyridine ones, we can notice a shift of 8 cm^{-1} to longer wave number side. This fact have allowed us to correlate each pair of bands to one conformer of the aliphatic chain of the DFP or FPPy molecules. These conformers are identified as GG (544 cm^{-1} for DFP and 552 cm^{-1} for FPPy), AG (556 cm^{-1} for DFP and 564 cm^{-1} for FPPy) and AA (570 cm^{-1} for DFP and 578 cm^{-1} for FPPy)(6-9), as shown in the table 2, and indicated in the figure 1.

The normal mode ν_{9b} generally has shown up as a weak Raman line and a medium intensity band in the infrared spectrum(10). Its wave numbers were assigned at the region of 230 cm^{-1} for many alkylbenzenes(6-9). We have observed three bands in this region, at the wave numbers of 206 cm^{-1}, 214 cm^{-1} and 230 cm^{-1}, as shown in the figure 8, with medium intensity, which are assigned to the conformers GG, AG and AA, respectively. These bands are almost insensitive to pyridine ring substitution, indicating that the strenght of the bonding ring-substituent as well the steric effect of benzene or pyridine rings are almost the same in both molecules.

The influence of the conformational structure of the aliphatic chain on the wave number of the normal mode ν_{10b} is more complex(6-9). In the case of some alkylbenzenes it was observed that the band at 184 cm^{-1} is coupled with the torsion of the methyl group and it was assigned to the normal mode ν_{10b} due to the conformer with four C-C bondings in a trans configuration. We have observed, as shown in the figure 8, a medium intensity infrared band at 181 cm^{-1} (6-9). Since we don't have a methyl group in the existant molecules, this band is assigned to the conformer AG(7) of the DFP and FPPy molecules, with overtone at the wave number of 363 cm^{-1}. One other band was observed at 151 cm^{-1} related to the normal mode ν_{10b} from terminal phenyl group of the gauch conformation the chain(6-9). These two bands were observed in the meso isomer of the 2,4-diphenylpentane(7) and they are assigned to the normal modes ν_{10b} from the conformer AG. It was also observed(6-9) at 163 cm^{-1} one band which was assigned to the configuration of the chain with all trans conformation of the chain. As shown in the figure 8, we have observed one medium-weak intensity band in the infrared spectrum of DFP, at 323 cm^{-1}, which is assigned to the overtone of the normal mode ν_{10b} from the conformer AA or GG, as in the case of the racemic conformers of the 2,4-diphenylpentane(7).

3.3. Vibrational Normal Modes from the Aliphatic Chain

Stretching CH vibrations

These are three symmetric and three antisymmetric CH stretching vibrations from the methylenic groups of the 1,3-disubstituted propanes. Differ-

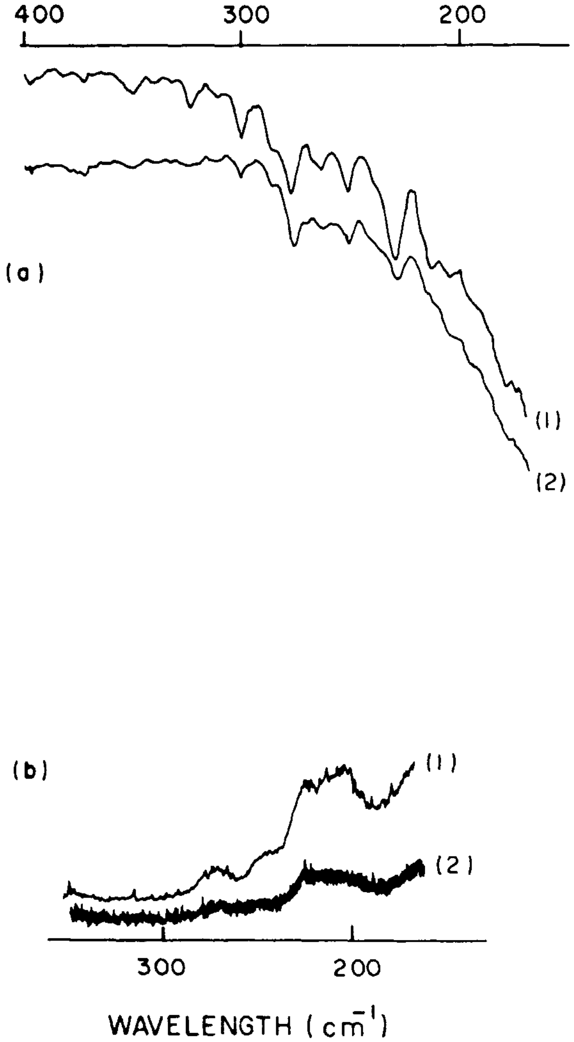

FIGURE 8. Infrared (a) and Raman (b) spectra of DFP (1) and FPPy (2) in the range of 400-200 cm^{-1}.

ently from the 1,3-dihalopropanes(21-23), which had shown an accidental degenerescency of some of these normal modes, the Raman spectra of the DFP and FPPy have allowed us to assign six wave numbers from CH stretching vibrations, in the region of 3000 cm^{-1} to 2850 cm^{-1}, as shown in the figure 2. The assignment of the wave numbers have been done considering that the high intense infrared bands are due to the antisymmetric CH_2 stretching vibrations and the high intensity Raman bands are due the symmetric ones. These assignments were shown in the table 3.

C-C stretching vibrations

There are two kinds of C-C stretching vibrations from the aliphatic chain of the DFP and FPPy: 1. the antisymmetric stretching which are medium intensity bands in the infrared spectrum and 2. the symmetric stretching which are low intensity bands. The wave numbers of these vibrations are dependent of the conformation of the chain(24,25). It was observed in the infrared spectra of DFP and FPPy three medium intensity bands at 1073 cm^{-1}, 1064 cm^{-1} and 1040 cm^{-1}, which are assigned to the antisymmetric stretching from the GG, AG and AA conformers, respectively. Only one band from the symmetric vibration can be assigned, at the wave number of 1018 cm^{-1}, as a shoulder at the lower wave number side of the normal mode ν_{18a} from the benzene ring.

CH_2 methylenic groups bending

There are four types of bendings from the methylenic groups, as known as: scissoring, wagging, twisting and rocking vibrations(10).

The scissoring vibrations were observed at the region of 1460-1420 cm^{-1} (24,25), the same region of many other vibrations from the benzene and pyridine rings. We could assign three bands at the 1458 cm^{-1}, 1444 cm^{-1} and 1436 cm^{-1} for both DFP and FPPy as being the scissoring vibrations by comparison of

TABLE 3. Vibrational assignments of the normal modes from the aliphatic chain of the DFP and FPPy.

Normal mode	$\bar{\nu}_{cm}$-1 (FPPy, DFP)			PS(1)		
$\nu^{a}_{CH_2}$	3001 (DFP), 2990 (FPPy)	2974 (DFP)	2928	2998	2975	2920
$\nu^{s}_{CH_2}$	2905	2894	2856	2898	2848	
ν^{a}_{CC}	1073	1064	1040	1082		
ν^{s}_{CC}	1018					
S_{CH_2}	1458	1444	1436	1450		
w_{CH_2}	1353, 1348	1338, 1320	1271, 1260			
t_{CH_2}	1297, 1290	1198, 1188	1148, 1135			
R_{CH_2}	866, 858, 845	807, 797, 783	751, 736, 727	840		
β_{CCC}	287 (GG),	277 (AA),	264 (AG)	330		
β_{HC} ring	596 (DFP)	600 (FPPy)				

ν = stretching, a = antisymmetric, s = symmetric, S = scissoring, t = twist, w = wagging, R = rocking, β = bending.

their infrared and Raman spectra. These comparations have allowed us to observe that while the bands due to the CC stretching vibrations are strong bands in the infrared spectra and weak in the Raman, as shown in the figure 4, the scissoring vibrations are observed as medium intensity in the Raman spectra.

It had been observed that the wave numbers of the wagging, twist and rocking vibrations are dependent on the conformation of the aliphatic chain(11,24-26). This fact brings in a new kind of complications in the infrared and Raman spectra of DFP and FPPy, since the twist and wagging vibrations are low intensity bands and the region of their wave numbers are the same as many other normal modes of the benzene and pyridine rings. But, even with these complications the comparison of the infrared and Raman spectra of both molecules, as shown in the figure 4, have allowed us to assign the wagging vibrations as a set of three pairs of bands, at the wave numbers 1353 cm^{-1} and 1348 cm^{-1}, 1338 cm^{-1} and 1320 cm^{-1} and 1271 cm^{-1} and 1260 cm^{-1}. An equivalent assignment was done with the twist vibrations and the correspondent wave numbers are: 1297 cm^{-1} and 1290 cm^{-1}; 1198 cm^{-1} and 1188 cm^{-1}; and 1148 cm^{-1} and 1135 cm^{-1}. Each pair of these wave numbers are from one type of vibration of the three stable conformers, but we are not able to assign an unargueable set of wave numbers for each conformer.

In the case of the rocking vibrations it was observed, like for 1,3-dichloro propane(11), three set of bands which have been assigned to these vibrations from each stable conformer. These wave numbers are: 866 cm^{-1}, 858 cm^{-1} and 845 cm^{-1}, which can be overlapped with the ν_{10a}, ν_5 and ν_{11} normal modes from the benzene and pyridine rings; 807 cm^{-1}, 797 cm^{-1} and 783 cm^{-1}, probably coupled with the normal mode ν_1 from the benzene ring; and 751 cm^{-1}, 736 cm^{-1} and 727 cm^{-1}, probably coupled with the normal modes ν_4 and ν_{11} from the rings. In each case, the identification of the wave numbers of these normal modes have been possible by comparing the wave numbers and intensities of each band from the infrared and Raman spectra for both molecules.

β_{CCC} angle bending vibrations

The wave numbers of these vibrations are also dependent on the conformations of the aliphatic chain(6-9,11,12). The bands observed for these normal modes are medium-weak intensity in the infrared spectra and they have been assigned, in order of increasing intensities, to the following conformers: GG at 287 cm^{-1}, AG at 264 cm^{-1} and AA at 277 cm^{-1}. This order of intensities is the same as observed for the normal modes ν_{9b} and ν_{16b}, from the pyridine and benzene rings. In the case of FPPy, these bands are shift to the low wave numbers side to 279 cm^{-1}, 257 cm^{-1} and 270 cm^{-1} respectively, as shown in the figure 8.

It was observed one strong intensity band in the infrared spectra of DFP at 596 cm^{-1} and FPPy at 600 cm^{-1}. This band was observed for syndiotactic crystalline 2,4,6,8-tetraphenylnonane(9), but no assignment was done. This band couldn't be observed in the case of isotactic polystyrene in the quenched or annealed forms, but one band in this region was observed in the case of the crystalline form(5). Although this band had also been observed for other molecular systems(11,12), no precise assignment was done. Our results have indicated that the wave number of this normal mode are dependent on the substituent of the aliphatic chain as well of the crystalline state of the molecular system(5,9,11,12), but it is independent on the conformation of the aliphatic chain, since only one band has been observed in each case. We have tentatively assigned this wave number to the H-C_{α}-ring angle deformation, which are decoupled with other molecular motions only in a rigid system, like in the crystalline state, or in molecules without long chain or with other terminal substituents. In these cases, this normal modes are coupled with other angle deformations from the aliphatic chain and it is observed one band at 350 cm^{-1} (6-9).

SUMMARY AND CONCLUSIONS

As we can see in the tables 1 and 2, the wavelengths of the normal modes from the benzene ring are close to the values of the polystyrene molecules(1).

The same results have been obtained with the wave numbers of the normal modes from the pyridine ring and those from the poly-(4 vinyl pyridine)(27). These facts indicate that the infrared and Raman spectra of these molecular models are very usefull in the assignment of the vibrational modes for these two polymers.

The analysis of the conformational structure of these molecules have indicated that there are three stable conformers in the liquid state and the stability order may be of the AA, AG and GG conformers, the same as observed in the 3-halo propyl benzenes(12), as shown by the normal modes ν_{9b}, ν_{10b} and ν_{16b} from the rings and β_{CCC} from the aliphatic chain. However, in the case of the polymers, the chain conformation are preferentially a trans configuration related to the aliphatic chain, with the phenyl groups perpendicular to the chain(6-9), as in the case of the GG conformers. These results indicate a strong compromise between the steric effects of the substituents of the alkyl chain, in establishing the final stable conformation. The energy calculations from these three stable conformers of the DFP and FPPy are in progress.

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