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Infrared Absorption Band Assignment in Benzanilide and Some of its p-Substituted Derivatives

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ABSTRACT

An attempt has been made to carry out a complete infrared band assignment for the infrared spectra of benzanilide and its p-methyl, p-chloro, p-bromo, p-carboxy, and p-nitro derivatives. Out of the six characteristic Amide Bands which originated from coupled vibrations of the peptide linkage- CONH–, four bands (Amide I, II, III and V) have been assigned for all the compounds studied. Aimide IV band was assigned for the unsubstituted benzanilide and p-nitrobenzanilide only. However, no absorption band(s) that can be readily attributed to Amide VI mode was observed for all the benzanilides.

Keywords: Benzanilide, IR Absorption Band

INTRODUCTION

The infrared absorption spectra of a number of amides have been investigated and complete vibrational assignments and normal coordinate analysis have been carried out on some of them (Velu *et al.*, 2011, Iheva, 1991 and Ufaruna, 2006). For secondary amides a maximum of six characteristic absorption bands have been shown to originate specifically from coupled vibrations of the peptide linkage, -CONH-. These are respectively referred to as Amide I, II …, VI Bands. Previous studies have identified bands located at 1655, 1529, 1322, 755, 725 and 600cm^{-1} with Amide I, II,…, VI modes respectively (Bellamy, 1968., Miyazawa *et al.*, and Geifer, 1966). Whereas Band I is almost entirely due to the carbonyl stretching absorption, II and III Bands arise from strong coupling between C-N stretching vibration and the in-plane deformation of the N-H group. Whilst IV-VI Bands are low frequency vibrations below 800cm^{-1}, it has not always, however, been possible to identify all these characteristic amide bands owing to the fact that Bands IV, V and VI normally appear in region where there are strong aromatic absorptions. In addition, their frequencies are affected by the type of substituents on the amide linkage (De Klein., 1972). It has also been found that apart from Band IV, these bands are sensitive to temperature and physical state in a number of N-alkylacetamides (Miyazawa *et al.*, 1956). Out of the compounds being studied in this work, Amide I and II Bands have been reported for benzanilides in chloroform (Rao *et al.*, 1971). While in the solid state I, II and II Bands have been assigned for benzanilide and 4^1-nitrobenzanilide (Geifer, 1966). In this study, an attempt has been made to carry out a complete infrared band assignment for the following compounds with the basic structure as shown. (Fig.I):

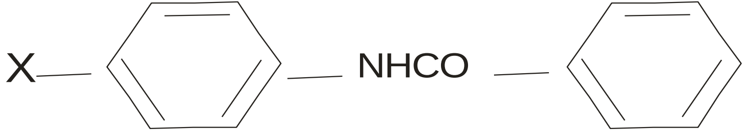

Fig. 1. The Molecular Structure of Benzanilide.

(where X = H, methyl, chloro, bromo, carboxyl, and nitro groups).

The assignment has been made possible by correlating the observed infrared absorption frequencies of these compounds with those of N-methylacetamides (Miyazawa *et al.*, 1958), ortho-methyl formanilide (De Klein, 1972), N-haloacetamides (D Klein and Plesman, 1972), and diketopiperazine (Miyazawa *et al.*, 1956). The assignments of absorptions arising from the benzene ring vibrations have been aided by those reported for aniline (Evans, 1960), and mono substituted benzenes (Whiffen, 1956., Green *et al*., 1961)

MATERIALS AND METHODS

All these reagents used were obtained from British Drug Houses Ltd. (BDH). P-Toludine, p-chloroaniline, p-nitroaniline, p-amino benzoic acid, and p-bromoaniline were recrystallised from alcohol while benzoic acidwas recrystallised from hot water. Acetic anhydride (Analar grade) was used without further purification. ThionyI chlorine (Laboratory grade, BDH) was redistilled.

All the benzanilides investigated in this work are listed in Table 1. Laboratory grade benzanilide (BDH) was recrystallised from water-methanol mixtures and dried in a vacuum desicator. All the other benzanilides were synthesized using the Schotten-Baumann method of benzoylation (Arthur, 1971). Equimolar proportions of the amines, chorides and ten percent (10%) aqueous sodium hydroxide with a slight excess of both the chlorides (10-15% above the theoretical value) and alkali were used. BenzoyI choride was synthesized from benzoic acid and thionyI chloride and the pure liquid was collected between 194-198^{0}C (Arthur, 1971) In the case of p-carboxybenzanilide, a slightly different procedure of benzoylation of aromatic amines was adopted in order to protect the carboxyl group (Arthur, 1971). BenzoyI acid and thionyI chloride and the pure liquid was collected between 194-198^{0}C (Arthur, 1971).

The micro analyses of all the anilides prepared were carried out at the micro-analytical laboratory in the University of Ibadan. The capillary tube melting point method was used to determine the melting point of the anilides.

The spectra of KBr pellets containing between 0.5 and 2mg of sample in about 150mg dry KBr and NujoI mulls of the samples were recorded on a perkin Elmer 577 spectrophotometer from 4000 – 200cm^{-1} at 15mins. scan. The instrument was calibrated with a polystyrene film. The infrared spectra of the solutions of the compounds were recorded on the same instrument in the 1750- 1600cm^{-1} region only. Spectroscopic grade chloroform (BDH) was used without further purification. Benzene (Analar grade, BDH) and dichloroethane (Laboratory reagent grade, BDH) were dried with anhydrous calcium chloride overnight before they were redistilled for use. The infrared (IR) frequencies reported in this work are believed to be correct $\pm$4cm^{-1} in the 4000-2000cm^{-1} and $\pm$ 2cm^{-1} in the 200-200cm^{-1} and $\pm$2cm^{-1} in the 2000- 200cm^{-1} region.

Table 1: Physical and Analytical Data on Benzanilide and Some of their Substituted Derivatives.

Names of Compound	Molecular Formula	Colour	Melting point (°C)	Calculated (%)				Found (%)			
				C	H	N	X	C	H	N	X
Benzanilide	$C_6H_5NHCOC_6H_5$	Light grey	160-162	70.16	5.62	7.10		77.94	6.28	6.78	
4-Methylbenzanilide	$CH_3C_6H_4NHCOC_6H_5$	Colourless	157-159	79.59	6.20	6.63		79.83	6.70	6.42	
4-Chlorobenzanilide	$CI\text{-}C_6H_4NHCOC_5H_5$	Colourless	191-193	67.39	4.35	6.05	15.30	67.78	4.35	5.48	13.36
4-Bromobenzanilide	$Br\text{-}C_6H_4NHCO_6H_5$	Colourless	208-210	56.54	3.65	5.07		56.65	4.19	4.92	
4-Nitrobenzanilide	$O_2N\text{-}C_6H_4NHCOC_6H_5$	Ligth Yellow	200-202	64.46	4.16	11.57		64.71	4.18	1.26	
4-Carboxybenzanilide	$HO_2C\text{-}C_6H_4NHCO_6H_5$	Faint Yellow	288-289	69.70	4.60	5.81		68.88	4.51	6.06	

Key: (X = Cl)

Table 2: The Observed Frequencies (cm^{-1}) and Assignment of the Infrared Spectra of Polycrystalline Benzanilides.

X=H	CH_3	Cl	Br	CO_2H	-NO_2	Assignment
3343(vs)		3348(vs)	3333(vs)	3337(vs)	3336(vs)	}Bonded ʋNH
3302(sh)	330 (s)	3298(sh)	3295(sh)			2x1597
	3193(sh)					1587+1524
	3113 (w)	3101(vw)				ʋCH
304 (w)	3056(vw)	3057(vw)				ʋCH
	3033(vw)					ʋCH
	29115(m)					ʋCH_3
	2855 (w)					ʋCH_3
1655(sh)						
						} Amido I
1650 (vs)		1654 (vs)		1635 (sh)	1655(s)	
1644(sh)	1645(vs)	1648 (vs)	1646(vs)	1648(s)	1649(s)	
1632(sh)	1637(sh)	1637(sh)	1637(sh)	1637(w)	1638(sh)	
					1615(m)	ʋNO_2
1599(s)	1597(s)	1596(s)	1592(s)	1592(m)	1597(s)	ʋNO_2
1575(m)	1508(w)	1579(m)	1580(m)		1581(m)	ƱC=C
1525	1524(sh)					
1522		1514(vs)	1514(vs)			Amid II
1501(sh)	1508(vs)	1505	1505(m)	1507(s)	1504(s)	
1485(w)	1490(m)	1487(s)	1487(s)		1483(vs)	ƱC=C
1468(sh)	1470(sh)	1469(sh)	1470(sh)			
		1443(sh)	1447(w)		1444(w)	ƱC=C
1433(vs)						2x714
	1402(s)				1406(s)	ʋNO_2?
			1391(vs)			ʋNO_2(symm)
		1355(vw)	1347(m)			
1326(w)						
1319(vs)	1317(s)	1314(s)	1312(s)	1320(m)	1309	
1300(w)	1297(m)	1303(sh)				Amide III
		1289(m)	1289(m)	1291(m)	1292(s)	
1261(m)	1266(m)	1255(s)	1260(s)	1254(w)	1259(vs)	
		1240(s)	1243(s)		1250(vs)	
1175(w)		1178(m)	1181(m)	1178(m)	1180(vs)	βC-H
1162(vw)		1160(vw)	1160(vw)		1161(vw)	βC-H
		1093(vs)	1101(vw)	1103(vw)	1113(vs)	
1075(w)	1974(vw)	1075(m)	1075(s)	1077(ww)	1075(m)	βC-H
1025(w)	1027(vw)	1021(w)	1028(vw)		1031(m)	βC-H
					1024(vw)	
		1011(s)	1010(s)			2x505(ʋN-C_6H_5) Ring
		998(vvw)	1002(sh)		1002(m)	
		968(w)			977(vw)	
927(vw)		928(w)	930(w)	923(w)	931(m)	ϒCH
910(vw)	902(w)	900(w)	902(vw)	903(w)	904(s)	ϒCH
885(vw)		895(m)				
					866(s)	
				853(m)	850(vs)	NO_2
					837(m)	
	813(s)	824(vs)	821(vs)		820(s)	ϒCH
791(nw)	799(w)	794(m)	795(m)	799(sh)	797(m)	

H-H	**CH_3**	**Cl**	**Br**	**CO_2H**	**$-NO_2$**	**Assignment**
				789(vs)		
				773(m)		
761(vw)						ϒNO_2' Amide IV?
748(vs)					751(vs)	Amides IV
716(vs)	714(s)	719(vs)	719(vs)	716(w)	722(s)	Amide V
		705(m)	701(sh)			
					697	
690(vs)	693(vs)	690(m)	693(w)	693(w)	692 (vs)	SφCCS
	676(w)		686(sh)		684(sh)	
	668(s)					
646(s)		648(s)	655(s)		657(vs)	α (CCC)
		642(s)			641(sh)	υC-CI
636(s)			631(vw)			
			616(vw)		617(vvw)	
598(w)						
				553(vw)		
	535(w)				534(vw)	NO rock
		517(s)	516(m)			υC_2-Br
513(m)	511(m)	508(m)	508(m)	493(sh)	510(s)	X-sens.
					504(sh)	
				450(s)		
		430(m)				
		420(sh)			420(m)	
			413(m)			φCC
			352(vw)			

Table 3: **CarbonyI Vibrational Frequencies (cm^{-1}) of Benzanilide and some of their Derivatives in the solid and Different Solvents.**

Solvent	Compound/Substituent X	XφNHCOφ	
		Solution	Solid
Benzene	$-CH_3$	1675	1645(vs) 1637(sh)
	-H		1650(s) 1644(sh)
	-CI		1654(vs) 1648(vs)
	-Br		1646(vs) 1637(sh)
	$-NO_2$		1655(s) 1649(s)
Chloroform	$-CH_3$	1680	1645(s) 1637(sh)
	-H	1682	1650(s) 1644(sh)
	-CI	1682	1654(vs) 1648
	-Br	1686	1648(vs) 1637(sh)
	$-NO_2$	1969	1655(s) 1649
1,2- Dichlorome-thane	$-CH_3$	1674	1645(vs) 1637(sh)
	-H	1673	1650(s) 1644(sh)
	-CI		1654(vs) 1648(vs)
	-Br		1646(vs) 1637(sh)
	$-NO_2$		1655(vs) 1649(s)
Acetonitrile	$-CH_3$		1645(vs) 1637(sh)
	-H	1665	1650(s) 1644(sh)
	-CI		1654(vs) 1648(vs)
	-Br		1646(vs) 1637(sh)
	$-NO_2$		1655(s) 1649(s)

Φ = PhenyI

Table 4: **Phenyl Ring Vibration of Benzanilide and their Derivatives.**

Vibrational Mode	**4^I – X – Benzanilide**					
	X=H	**CH_3**	**Cl**	**Br**	**CO_2H**	**NO_2**
υCH	3073					
	3047	3056	3057			
	3003					
υCC	1599	1597	1596	1592	1593	1597
	1575	1580	1579	1580		1581
	1485	1490	1487	1487		
	1468	1470	1469	1470		
βCHS						
	1175		1178	1181	1178	1180
	1162		1160	1160		1161
	1075	1074	1075	1075	1077	1075
ϒCH	1025	1027	1021	1028		1031
	927		928	930	923	931
	910	902	900	902	903	904
		813	824	821		820
	791	799	794	795	799	797
φCC	690	693	690	693	693	692
				413		
α(CCC)						
	646		648	655		657

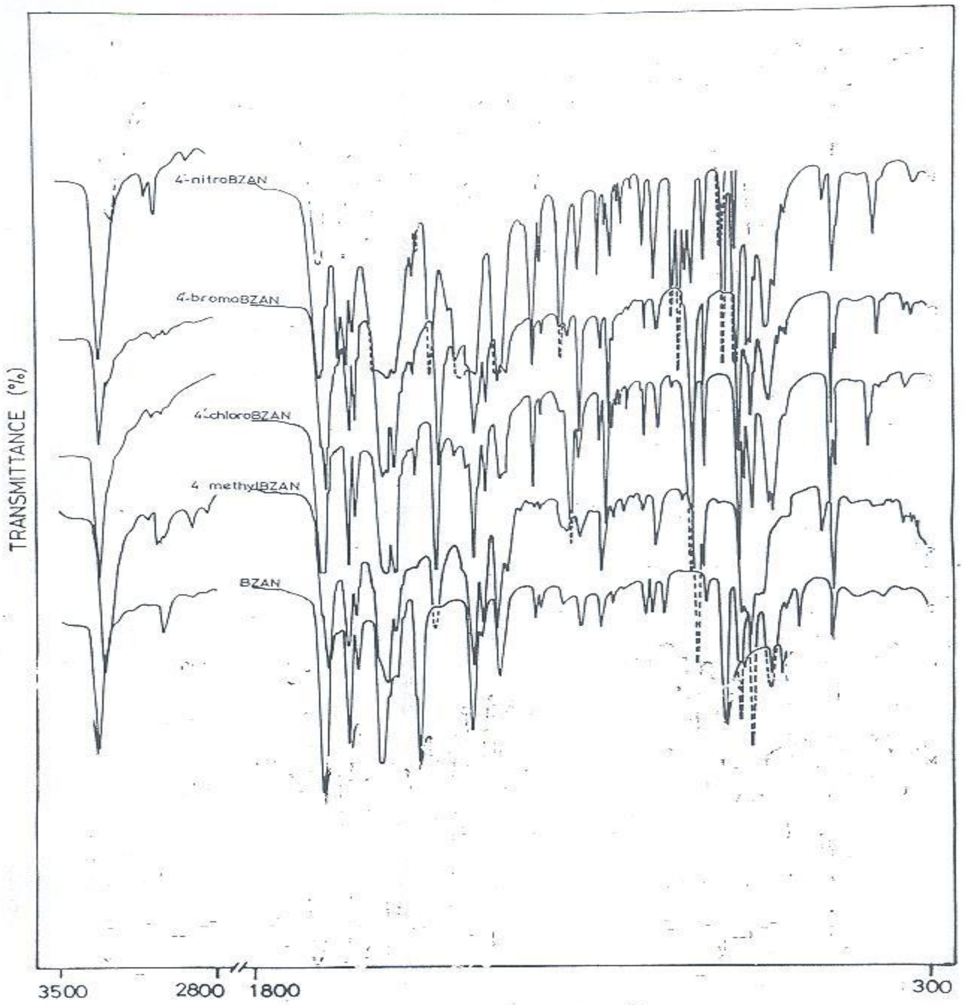

Fig.2. The KBr infrared spectra of polycrystalline benzanilides

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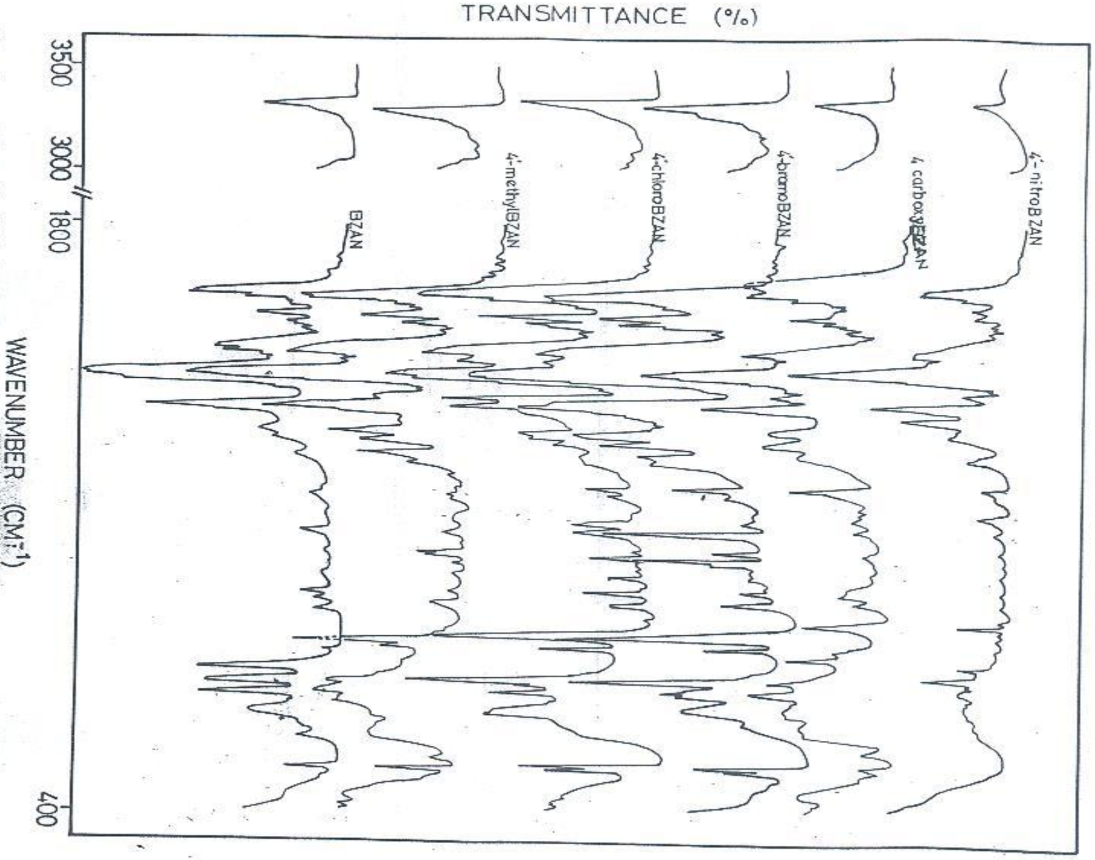

Fig. 3 The Nujol infrared spectra of polycrystalline benzanilide and some of its derivatives.

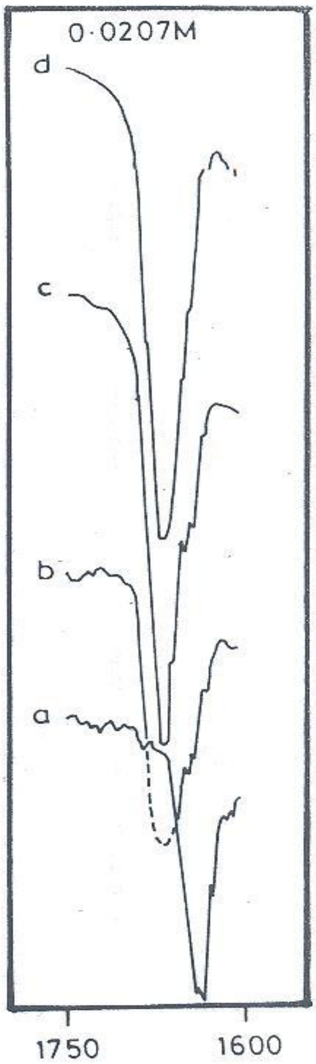

Fig.4 . Infrared carbonyl absorption band of benzanilides in (a) Nujol, (b) Benzene (c) 1,2-dichloroethane and (d) Chloroform.

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RESULTS AND DISCUSSIONS

Table 1 shows the results of the micro-analysis of the anilides synthesized as well as some of their physical properties. The agreement in values between the theoretical and the actual values found is satisfactory. The infrared spectra of polycrystalline benzanilides run in KBr pellets between 4000 and 200 cm^{-1} are shown in Fig. 2 while Fig. 3 depicts their infrared NujoI spectra. The agreement in the frequencies of absorption bands in the spectra of the benzanilides is satisfactory. The assignments of the fundamentals in the KBr and NujoI spectra are contained in Table 2. The infrared carbonyl absorption band of benzanilde in NujoI, benzene, 1,2-dicloroethane and chloroform are shown in Fig. 4.

BAND ASSIGNMENTS

Characteristic Amide Bands

Previous infrared study of bezanilide has led to the identification of the bands at 1655, 1529 and 1322cm^{-1} with Amide I, II and III modes respectively in the solid state (Geifer, 1966). In the present work, very strong bands located in the KBr spectrum of this compound at 1650, 1522 and 1319cm^{-1} can be assigned to these Amide modes respectively. The splitting of the Amide II band at 1525 and 1522cm^{-1} is not unusual. A similar behaviour of this mode has been observed for benzanilide in chloroform solution (Rao *et al*., 1971), and for most of the N-monosubstituted amides in the solid state (Bellamy, 1968). In the infrared spectrum of N-methylacetamide a strong band which appeared at 1299cm^{-1} was assigned to Amide III band with the aid of a normal coordinate analysis (Miyazawa, *et al*., 1958). Similar treatment of trans- ortho methylformanilide has led to the assignment of a series of bands at 1380, 1288 and 1262^{-1} to Amide III band (Siddall *et al*., 1968). It is therefore not unlikely that a weak infrared feature located at 1297cm^{-1} and a medium one at 1258cm^{-1} in the KBr spectrum of benzanilide can be attributed to the Amide III mode. Corresponding assignments of Amide I to III bands have been made for the other substituted benzanilides. It can be seen from Table 2 that the absorption frequencies for each of the Amide band in all the benzanilides lie within a close range.

Bellamy (Bellamy, 1968) reported a frequency of 620cm^{-1} for Amide IV absorption although it has been claimed that this mode should be close to 750cm^{-1} (Siddal *et al*., 1968). Only benzanilide and 4^{1} – nitrobenzanilide show absorption bands near 750cm^{-1}.

These are located at 748 and 751cm^{-1} respectively. Moreover none of the benzanilides studied have any absorption bands near 620cm^{-1}. Tentatively, the bands at 748 and 751^{-1} have therefore been assigned to amide IV. This conforms with a similar assignment at 758cm^{-1} in the spectrum of trans-ortho-methylformanilide (Siddall *et al*., 1968), but disagrees with a former assignment at 745cm^{-1} to the out-of-plane NO_2 deformation (ΥNO_2) (Siddall *et al*., 1968) in 4^{1} – nitrobenzanilide. It thus appears that the previous assignment of NO_2 in 4^{1} – nitrobenzanilide may now need to be revised since this mode (ΥNO_2) is most likely to be overlapped by the Amide IV band absorption.

The out-of-plane N-H vibration otherwise called Amide V Band, appears at 725cm-^{1} in both N-methylacetamide and O-methyI formanilide. Strong absorption now observed near 720^{-1} in the spectra of all the benzanilide derivatives can be associated with the Amide V mode.

The Amide VI mode which arises from the out-of-place vibration of the carbonyl group (Bellamy, 1968) has earlier been associated with a medium band near 600cm^{-1}in N-alkylacetamide (Miyazawa, *et al*., 1958, Miyazawa *et al*., 1956 and Siddall, *et al*., 1968). This band is usually of very weak intensity and seldomly observed (Siddall, *et al*., 1968). As can be seen (Table 2), no absorption bands that can be readily attributed to Amide VI mode is observed in all the benzanilides.

The nature of Amide II modewhich is of the carbonyl absorption is of interest. In the solid state this band appears either as strong singlets or doublets with a series of shoulders as indicated in Table 2. These features could be due to rotational isomerism (Nyquist, 1963), polymer groupings or crystal field effects (Bellamy, 1968).

In the solid spectra of benzanilide and its p^{1} – substituted derivatives, the υCO is centered around 1650cm^{-1}. It is obvious from Fig.4 and Table 3 that the carbonyl groups are all bonded in the crystalline phase as shown by the frequency lowering of υCO from solution to solid. Hence this band cannot be attributed to C=O monomers only. The predominance of crystal field effect in the solid state can also be ruled out since the characteristics features of the carbonyl absorption bands observed in solutions of chloroform, 1, 2, - dichloroethane and benzene are identical to those observed in the solid state spectra in frequency and structure even at varying solution concentrations and temperature and benzene are identical to those observed in the solid state spectra in frequency and structure even at varying solution concentrations and temperatures.

The NH stretching vibrations of secondary amides are known to absorb near 3440cm^{-1} in solution but shift to lower frequencies in the solid state due to hydrogen bonding. In the benzanilides under study, strong NH absorbtions have been observed near 3300cm^{-1} and have also been attributed to the bonded NH vibrations. These assignments are in conformity with reported values for similar molecules in the solid state (Bellamy, 1968).

PhenyI Ring and Substitutent Group Vibrations.

The assignment of the ring vibrations viz: υCH, υCC, βCH and υCH have been made by correlating observed spectra with those of related molecules such as aniline (Evans, 1960), biphenyl, stilbene and nitro and carboxylate groups (Green *et al*., 1961). As shown in Table 4, the frequencies of these vibrations are relatively unshifted in going from one molecule to the other. This would indicate that the phenyl ring vibrations are virtually unaffected by the peptide linkage in these benzanilides.

Two out-of-plane ring deformations (ϕCC) are expected for the benzanilides under study with one absorption near 698cm^{-1} (Whiffen, 1956) and the other at Ca. 405cm^{-1}. The strong bands which were observed in the IR solid spectra of these compounds near 690cm^{-1} have therefore been ascribed to the higher energy ϕCC mode. Only chloro-and bromobenzanilide show absorptions at 420(sh) and 413(m) respectively and these have been assigned to the second ϕCC mode. This band is probably overlapped by the medium NO_2, rocking vibration at 420cm^{-1} (Siddall *et al.*, 1968) in the spectrum of 4^1 – nitrobenzanilide.

With the exception of 4^1 – methyIbenzanilide all the compounds in this series possess strong peaks near 650cm^{-1}. The assignments of these to the in-plane deformations of the benzene ring (ȣCCC) which is straightforward is in satisfactory agreement with previous values reported for this deformation in other substituted benzene molecules (Green, *et al.*, 1961).

The characteristic carbon-halogen vibrations for the chloro- and bromobezanilides (υCC-CI and υC-Br) have been assigned, respectively, to the strong bands observed in the solid state at 642 and 514cm^{-1}. These frequencies satisfactorily fall within the predicted range (Bellamy, 1968).

Of the three vibrational frequencies of 4^1-nitrobenzanilide previously reported at 1342.5, 1530 and 745cm^{-1} and assigned to symmetric, asymmetric and out-of-plane deformation modes of the nitro group respectively (Exner and Sokaniova, 1972), only the lowest energy mode near 745^{-1} is now observed at 751cm^{-1} in the solid spectra of the compound. This has been attributed to the Amide IV Band. This has been shown in benzanilide to interact and possibly overlap with the Amide IV Band. The υCO absorption is found to split into doublet at 1678 and 1672cm^{-1}in the spectrum of solid p-carboxybenzanilide. Furthermore the vibrations at 789 (vs), 773 (m) and 450 (s) cm^{-1} in the spectrum of this carboxyl derivative are missing in the spectra of other benzanilides. It is therefore not impossible to attribute these vibrations as characteristic of the carboxyl group. The higher frequencies may be due to the in-plane bending vibrations of the CO_2H group while the 450cm^{-1} band probably correspond to the out-of-plane deformation of the carboxylates.

In the infrared spectrum of solid p-methyIbenzanilide, a band of medium intensity located at 2915cm^{-1} and a weak peak at 2855cm^{-1} have been respectively assigned to the asymmetric and symmetric vibrations of the methyl group. These assignments are in accord with those of previous studies (Bellamy, 1968). The possibility of attributing the only band near 1465cm^{-1} which is a shoulder at 1470cm^{-1} to CH_3 deformation vibration is ruled out as other members of the series exhibit similar features in their solid infrared spectra. It is therefore quite obvious that there is a strong vibrational coupling of the CH_3 deformations in this region with other fundamentals.

A few of the observed frequencies that cannot be accounted for in terms of fundamental transitions have been tentatively assigned to some possible combination and overtone bands as shown in Table 2.

CONCLUSION

Definitive assignments have been made for four (Amide, I, II, III and V) out of the six characteristic Amide Bands expected for the peptide linkage in each of the benzanilides investigated in this study. Amide IV mode has been assigned for the unsubstituted benzanilide only while no absorption band(s) could be attributed to Amide VI mode in the spectra of all the benzanilides. Furthermore, attempt has been made to assign most of the phenyl ring and substituent vibrations for all the compounds investigated.

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