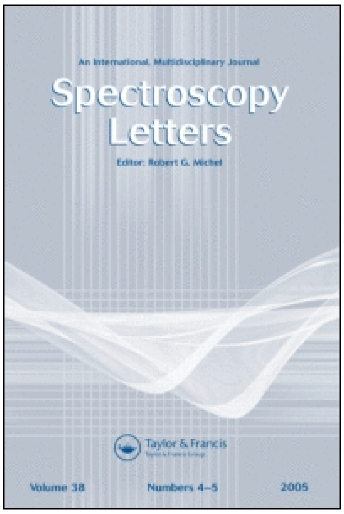

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INFRARED SPECTRA AND AM1 CALCULATIONS OF N-BENZYLIDENEANILINES

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INFRARED SPECTRA AND AM1 CALCULATIONS OF N-BENZYLIDENEANILINES

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ABSTRACT

The molecular structure and conformation of nine substituted N-benzylideneaniline $R1C_6H_4CH{=}NC_6H_4R2$ where R1=H, R2=OCH_3, CH_3 or Cl; R1=OCH_3, CH_3, Cl or NO_2; R2=H; R1=NO_2 R2=OCH_3 and R1=OCH_3 R2=Cl have been studied experimentally by FTIR spectroscopy and theoretically using the AM1 semi-empirical quantum-mechanical method. From IR data of substitued N-benzylideneaniline, a decrease in the C=N stretching frequencies were observed. There is a correlation between C=N stretching frequencies and the Hammett σ_R constant of substituents. The calculated values of torsional angle (θ_N) between the H-C=N plane and the N-phenyl ring of the compounds show that the stronger the electron withdrawing properties of the substituent, the larger the angle. There is

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also relationship between θ_N and Hammett σ_R constant of substituents. The dipole moments, bond order and electron density values of studied compounds have also calculated using semiemprical AM1 method.

Key Words: N-benzylideneaniline; Substituted N-benzylideneaniline; IR spectra; AM1

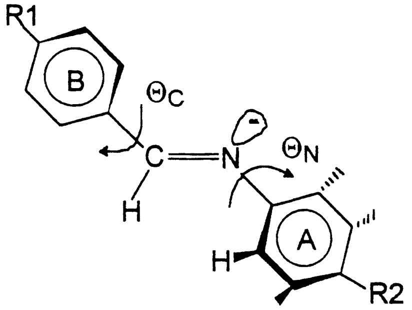
INTRODUCTION

Shiff bases play an important role in many fields of chemistry and biochemistry due to the biological activity they posses[1,2]. A model aromatic shiff base trans N-benzylideneaniline and their derivatives has been extensively studied over the years. The isoelectronic molecule N-benzylideneaniline is also the basic constituents of many compounds which show liquid-crystal properties[3]. The general structure of NBA and its derivatives studied are shown in Fig. 1.

There are several papers on the interpretation of the vibrational spectra of N-benzylideneaniline and its derivatives[4–10]. The most comprehensive experimental and theoretical data on the vibrational spectra of benzylideneaniline and its fluoroderivatives are presented in ref [8]. In ref [6] interpretations of vibrational spectra of the benzylideneaniline and p-p′-disubstituted benzylideneaniline are given. The molecular structure and conformation of benzylideneaniline and its derivatives has been studied other experimental tehniques such as ^{1}H and ^{13}C NMR[11–13], UV[14], gas electron diffraction method[15] and X-ray[16–18] and studied theoretically[8,10,19–21].

In this paper FTIR spectra of N-benzylideneaniline (NBA), seven monosubstituted and two disubstituted derivatives have been recorded. Vibrational assignment have been made for fundamental modes. It is difficult to interpret the spectra of these molecules because of their high complexity and low symmetry. The interpretation of the observed bands is based on the intensity of the bands and comparison with the assignments for related molecules.

The conformational behaviour of substitued NBA are investigated by semiemprical AM1 quantum mechanical calculation method. The dipole moment, torsional angles, bond order and electron density values of studied compound have calculated and discussed. The purpose of the present paper is to discuss the interpretation of the infrared data and understanding of the substituent effect on the conformational state.



1	R1=H	R2=H
2	R1=H	R2=OCH_3
3	R1=H	R2=CH_3
4	R1=H	R2=Cl
5	R1=OCH_3	R2=H
6	R1=CH_3	R2=H
7	R1=Cl	R2=H
8	R1=NO_2	R2=H
9	R1=NO_2	R2=OCH_3
10	R1=OCH_3	R2=Cl

Figure 1. Molecular model of N-Benzylideneanilines (NBA).

EXPERIMENTAL

All starting chemical used were reaged grade and used without further purification. All compounds, synthesized by refluxing equimolecular amounts of p-substitued benzaldehydes and p-substituedanilines in dry benzenes. The reaction was over in about 2 h. The solvent was removed by evaparation in vacuo and the residue was crystallized from ethanol or petroleum ether. Melting points of compounds were determined. The IR spectra of compounds were recorded between 4000–400 cm^{-1} on Mattson 1000 FT-IR spectrometer, which were calibrated using polystrene. The samples were prepared as mulls in nujol between CsI plates and KBr disc.

Method of Calculation

Geometry optimisation of NBA and its derivatives by the AM1 semi-emprical quantum-mechanical method[22], implemented with the MOPAC package[23] running on a Pentium 233 PC, was calculated starting from their crystallographic coordinates. Geomety optimizations of the structure of the compounds were carried out using the Fletcher-Powell-Davidson algorithm[24,25] implemented in the package and the PRECISE option to improve the convergence criteria. To determine the conformational energy, two conformational parameters were chosen, θ_N and θ_C from 0° to 90°, varied every 10°. At each point a full geometry optimization was carried out.

RESULTS AND DISCUSSION

The Discussion of Infrared Data

The IR and Raman data on NBA and its isotopomers was reported Meic and Baranovic[5] who gave approximate interpretations and selected values of phenyl group frequencies. Kozhevina et al.[8] carried out a normal coordinate analysis for the benzylideneaniline and its fluoroderivatives. Figueroa et al.[6] also reported IR data of p,p′- disubstitued N-benzylideneanilines. However their assignment of some modes were not agreement with Kozhevina et al[8]. We assigned the vibrations of NBA and substitued NBA by comparison with the assignment for mono and disubstitued benzene[26–29], and stilbene[30].

The NBA molecule contain two aromatic ring molecules. One of them is benzylidene ring and the other ring is aniline. In the stucture, two ring are connected through a azomethine (-CH=N-) group. It has 25 atoms and 69 fundemental frequencies. All the vibrations are infrared and Raman active. The observed frequencies of NBA and its derivatives together with the relative intensities, probable assignments and related data for comparison are given in Table 1. The IR spectra of NBA and three substitued NBA are shown in Fig. 2 as representative illustration. For nomenclature of the normal mode of vibration, a substituted benzene in para position (point group C_{2v}) was considered, while the Wilson nomenclature was maintained for the benzene ring vibrations.

Briefly, to simplify the interpretation of these complex spectra, the vibrations can be divided into three groups: phenyl ring (Ph) vibrations, vibrations of the CH=N and substituent group vibrations.

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Phenyl Ring Vibrations

For the monosubstitued phenyl ring 24 vibration are independent of the substituent and the other 6 are X-sensitive vibration. These vibrations are described as Ph-X stretching and bending vibration, in-plane and out-of-plane deformations. Their frequencies shift significantly with mass or inductive or mesomeric effects of the substituent, but also influence the absorption frequency a ring stretch, an in plane and out of plane ring deformation. These ring vibrations are coupled with the Ph-X vibrations in such a way as to make it difficult to determine which frequency belongs to a Ph-X vibrations and which frequency to a ring vibrations. It should be noted that the phenyl ring frequencies of NBA differ slightly from the monosubstitued benzene frequencies. For this reason, the IR data in Table 1 do not always agree completely with the assignments in the literature.

The benzene e_{2g} degenerate ring stretch (1596 cm^{-1}) is not greatly perturbed upon substitution and the two frequencies in the IR lie close to that for the benzene vibration. The e_{1u} degenerate vibration of benzene at 1486 cm^{-1} also split into two bands that are close to the original benzene frequency. We observed these bands at 1593, 1580, 1485 and 1452 cm^{-1} and assigned them to ring stretching vibrations of NBA (8a, 8b,19a and 19b, respectively corresponding to the Wilson notation[31]) 19a and 19b modes tend to show increases in frequency upon substitution (as a results of a preferential localization of the p-electron on the different CC bonds[32]).

The CH in plane vibrations derived from the two degenerate e_{2g} (1178 cm^{-1}, 9a, 9b) and e_{1u} (1075 cm^{-1}, 18a,18b) and two non-degerate b_{2u} (1156 cm^{-1}, 5) and a_{2g} (1326 cm^{-1}, 3) benzene vibrations. Upon monosubstitution the degerate e_{2g} benzene vibrations (No 9a, 9b) at 1178 cm^{-1} is perturbed and gives rise to a specific vibration of a medium intensity in the IR at ca 1170 cm^{-1} (No 9a) and to a nonspecific band at ca 400 cm^{-1} (No 9b). Therefore we assigned the 433 cm^{-1} band to 9b Wilson mode in disagreement with the assignment of Kozhevina et al[8].

The CH out of plane bending vibrations derived from the two non-degerate b_{2g} (995 cm^{-1}, 5) and a_{2u} (673 $cm^{-1,}$ 11) and two degerate e_{2u} (975 cm^{-1}, 17a, 17b) and e_{1g} (849 cm^{-1}, 10a, 10b) benzene vibrations. We observed 8 bands in the region 990–820 cm^{-1} which contein azomethine group vibrations and assignments are given in Table 1.

The stronger CH in-phase out of plane deformation band (γ(CH) 11 or umbrella mode) occurring in the region ca 770 ± 50 cm^{-1} also tends to shift in frequency with the substituent. Kozhevina et al.[8] assigned the IR band at 700 cm^{-1} as a CH out of plane deformation mode (Wilson mode 11). However we observed at 749 cm^{-1} to the γ(CH) 11 mode in agrement Meic and Baranovic[5] and Figueroa et al[6]. The 749 cm^{-1} band shifted to higher

Table 1. Observed Vibrational Frequencies (cm^{-1}) and Assignments for N-Benzylideneanilines

Assignment		1[a]	1[b]	1 (our)	2	3	4	5	6	7	8	9	10
ν(C=N)		1633vs	1625s	1629ms	1624m	1630m	1627s	1623w	1632ms	1629m	1619mw	1622mw	1619w
ν_{ring}	8a	—	—	1621sh	1605vw	1605w	1601w	1606m	1611m	1622m	1606m	1603mw	1606m
ν_{ring}	8a	1590s	1590s	1593m	—	1598w	—	1590m	1590s	1591m	1590w	1597m	1590w
ν_{ring}	8b	1580s	1575m	1580m	1577mw	1579m	1578m	1577m	1576m	1578m	1575w	1575w	1575w
ν_{ring}	19a	—	—	1506vw	1506mw	1506vs	1506w	1512m	1512m	1506w	1513mw	—	1513mw
ν_{ring}	19a	1483s	1480s	1485w	—	1489vw	—	1495vw	1485m	1492m	—	—	—
ν_{ring}	19b	1450s	1450s	1457m	1456w	—	1456w	—	—	1456w	—	—	1460w
δ(C-H$_a$)		1366m	1365m	1366m	1366w	1366w	1366w	1366w	1366sh	1366w	1366w	1366w	1366w
δ(C-H)	3	1316m	1310m	1311w	1311w	1311m	1312m	1308m	—	1320vw	1311w	1322w	1311w
ν_{ring}	14	1291w	1295w	—	1297vw	1291vw	1296mw	1301m	1292vw	1298vw	—	1294w	—
ν(C-Ph)		—	—	1235w	1246m	1247w	1236w	1251m	1241w	—	1256mw	1249s	1256mw
ν(N-Ph)		1198s	1190s	1191m	1191w	1192s	1191m	1193w	1192m	1189m	1190w	1192w	1190w
δ(C-H)	9a	1178m	1165s	1168s	1169vw	1169m	1163mw	1165m	1173m	1168m	1163mw	1161mw	1163mw
δ(C-H)	15	1158sh	1155sh	1156vw	1156vw	1156vw	1156w	1153w	1154w	1156w	—	—	—
δ(C-H)		—	—	1106w	1109w	1108w	1110w	1107mw	1106m	1125w	1107w	1112mw	1107w
δ(C-H)	18b	1066m	1070m	1072mw	1072w	1071w	1072m	1074mw	1073m	1074m	1071m	—	—
δ(C-H)	18a	1025m	1020m	1026w	1029m	1025w	1025w	1033m	1024w	1023w	1026m	1036m	1026m
ν_{ring}	1	1000w	997w	1001vw	1008vw	1000w	1011m	—	998w	1011m	1009w	1013w	1009w
γ(C-H)	17a	991w	985m	987w	—	—	992vw	—	980m	991vw	—	—	—
γ(C-H$_a$)		975m	970s	972m	969vw	970mw	976m	968w	—	969ms	978	970w	978

γ(C-H)	17b	925m	920m	923vw	917vw	–	920mw	–	–	–	919	918w	919
γ(C-H)	10a	908m	903s	905mw	–	914w	–	909mw	908m	910s	–	–	–
Azomet.vib.		875	865m	872mw	882m	882m	882m	878mw	877m	889vw	887w	892m	887w
γ(C-H)	10b	830vw	830w	830w	834vs	826m	833m	835vs	833vw	829vs	839s	838m	839s
γ(C-H)	10a		820vw	820vw	–	813vs	822s	820m	814vs	–	820w	821m	820w
δ_{ring}(X-sens)	12	766vs	764sh	764vs	–	–	–	771m	773m	782sh	767w	761m	767w
γ(C-H)	11	–	758s	749w	759m	754s	756s	757m	752s	761s	744m	749ms	–
	–	–	–	–	720s	709m	713m	721s	711m	711s	721s	720s	722m
γ_{ring}(X-sens)	4	700vs	690vs	693vs	690s	690s	689s	693s	693s	694s	680m	690m	680m
δ_{ring}		671vw	663vw	–	668vw	668vw	668vw	668w	668sh	668vw	668w	669w	669w
δ_{ring}		658w	645w	651w	–	–	631w	–	642w	–	636w	637w	636w
δ_{ring}	6b	617w	620w	618vw	–	625w	593mw	619m	–	585mw	–	–	–
γ_{ring}	16a	541s	540s	541m	541m	536s	533vs	531m	539s	539vs	543m	549s	538m
δ_{ring}	6a	533m	–	529mw	535w	–	–	–	531m	–	525m	530w	–
γ_{ring}	16a	518m	520m	517w	–	516vw	516vw	510w	517m	518vs	511w	504w	500vw
		–	–	–	–	458w	453m	–	456m	458s	446vw	454w	446vw
δ(C-H)	15	436m	433m	433w	–	–	425m	–	–	431m	–	442w	–
γ_{ring}	16b	–	410w	418vw	–	419vw	–	419w	419w	409w	419w	–	419w
ν_{as} NO$_2$											1538m	1530m	
ν_s NO$_2$											1339w		
δ NO$_2$											856m	850vs	
ν(Ph-R)							1098m			1099m	1093m	1102m	1093m
							1090s			1090s			
ν(O-CH$_3$)					1042m			1040w					

[a,b] Taken from refs. [6,8], respectively. vs: very strong, s: strong, m: medium, w: weak, vw: very weak, sh: shoulder.

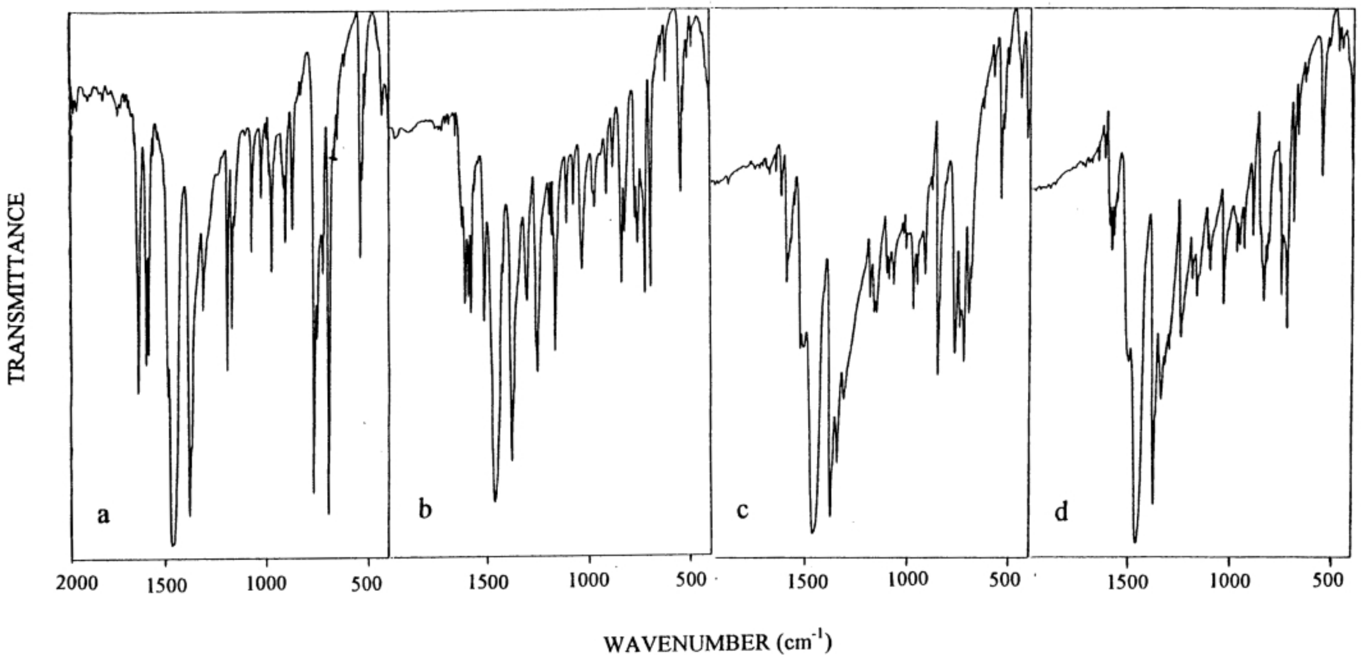

Figure 2. The infrared spectra of NBA (a) metoxybenzylideneaniline, (b) nitrobenzylideneaniline, (c) and nitrobenzylidenemetoxyaniline (d) in the range 2000–400 cm^{-1}

frequencies in the IR spectra of all of substitued benzylideneanilines except for nitro substituent which in frequency shift occurs to lower wavenumbers.

We observed two strong and weak bands at 693 cm^{-1} and 668 cm^{-1} , respectively in the IR spectrum of NBA. The 693 cm^{-1} band slightly shifted to lower frequency upon substitution. The 668 cm^{-1} band however did not display any shift. Therefore we assigned the 693 cm^{-1} band to γ_{ring} (No 4) in agreement with the assignment of Meic and Baronovic[5]. The 668 cm^{-1} band is assigned to δ_{ring} vibrations of phenyl ring.

We observed a weak band at 410 cm^{-1} in the IR spectrum of NBA which is shifted to higher frequency upon substitution and assigned to γ_{ring} vibrations of phenyl rings. The other phenyl vibrations observed in the IR spectrum of NBA are assigned in agreement with Kozhevina et al[8]. The number of CH stretching vibrations decreases for mono- and disubstitued NBA while 10 aromatic frequencies were expected for NBA in the 3100–3000 cm^{-1} region. The bands observed in this region are assigned to CH stretching vibrations.

CH=N Group Vibrations

The C=N stretch (ca 1630 cm^{-1}) is the most characteristic band of the azomethine group and good group vibration. The intensity varies from moderate to strong and the band is generally sensitive to conformation. The IR band at 1629 cm^{-1} is assigned to the C=N stretching mode. As inferred from Table 1, this band shifted to higher frequencies in the IR spectra of compounds 3 and 6 and lower frequencies for the other compounds studied. The slight changes are observed for the intensities of these bands. Intensity changes occur through the azomethine group and benzene ring conjugation effect[33]. However Kozhevina et al.[8] belived to the change in π-conjugation of the azomethine group and the benzene rings is insignificant according to the normal coordinate analysis. Chances in molecular structure, especially those in twist angles of the aromatic rings (due to different influence of substituents) (Table 2) are expected to affect the π-electron distribution across the system. This will reflect on the IR band position. In previous paper[6] it was pointed out that increasing the donor or acceptor properties of the para substituent decreases C=N stretching frequency. The C=N stretching frequency have been correlated with different types of Hammett constant. The best correlation was found for the Hammet σ_R constant (for an electron-donating or electron-withdrawing group is introduced into the para position of the benzylidene ring), as is shown in Fig. 3. It was found that the resonance effects of substituent prevail over the inductive ones. This is accordance with results from AM1 MO calculation. The Hammett relation is not obtained for the p-aniline ring substituent. In such case a

Table 2. Phenyl Rings Torsional Angles, Dipole Moments, Atomic Charge Densities, and HOMO Energy Levels in N-Benzylideneanilines as Obtained from Semiempirical AM1 Calculations

			θ_N(°)		θ_C(°)		μ(D)				
No.	R1	R2	Exp	Calc.	Exp	Calc.	Exp	Calc.	qN	qC	HOMO (eV)
1	H	H	55.2[a] 52[b] 36[c]	36.2	−10.3[a] 0[b] 0[c]	4.67	1.57[d]	1.39	−0.1497	−0.0094	−8.904
2	H	OCH_3	–	31.22	–	6.33		0.69	−0.1446	−0.0173	−8.541
3	H	CH_3	–	33.85		4.96	–	1.32	−0.1486	−0.0117	−8.739
4	H	Cl	–	33.98	–	3.59	–	2.23	−0.1528	−0.0033	−8.937
5	OCH_3	H	–	36.96	–	4.56	–	0.675	−0.1571	−0.0014	−8.685
6	CH_3	H	–	34.86	–	3.56	–	1.54	−0.1522	−0.0073	−8.806
7	Cl	H	–	35.89	–	6.22	1.79[d]	1.77	−0.1456	−0.0132	−8.972
8	NO_2	H	–	34.09	–	4.02	4.20	5.99	−0.1292	−0.031	−9.38
9	NO_2	OCH_3	37.9	28.38	–	12.30		6.51	−0.1179	−0.0439	−8.968

[a] From X-ray[18].
[b] from gas electron diffraction[15].
[c] from PES[38] and [d] from[39].

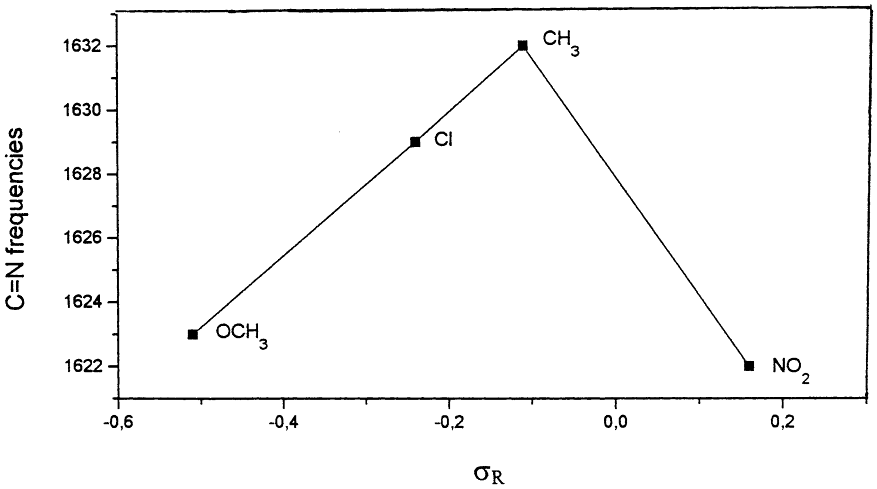

Figure 3. Plot of ν(C=N) frequencies vs. Hammett σ_R constants in 5–8.

trend to a general coplanarity should be favoured (it might be considered that steric hindrance effect of the aniline ring is significant).

Kozhevina et al.[8] assigned IR bands at 1198 cm^{-1} and 1178 cm^{-1} to the N-Ph and C-Ph stretching modes, respectively. The former mode was assigned to the IR band at 1193 cm^{-1} and the latter to one at 1233 cm^{-1} in ref. [34]. Figueroa et al.[7] assigned these modes at 1310 cm^{-1} and 1190 cm^{-1}, respectively. We observed a medium band at 1191 cm^{-1}, a strong band at 1168 cm^{-1} and two weak bands at 1235 cm^{-1} and 1311 cm^{-1}. As inferred from Table 1, the IR band at 1235 cm^{-1} shifted to a higher frequency upon substitution. However, the 1168 cm^{-1} and 1310 cm^{-1} bands slightly shifted. It was not possible to make here a straightforward assignment of C-Ph stretching mode. The Ph-C stretching vibration in alkyl benzenes appears weakly in the neighbourhood of 1210 cm^{-1}. This band shifts to higher frequencies in benzenes substituted with atoms with an unshared pair of electrons next to the ring such as nitrogen[35]. Therefore we tentatively assigned the 1235 cm^{-1} band to C-Ph stretching mode.

Calculation Results

Structural studies confirm the nonplanar conformation of the NBA molecule in the solid[18], in the gas phase[15] and in solution[11]. The conformation of molecule has been reported to be influenced to great extent by the properties of substituents to the aromatic rings[36]. The insertion donor or acceptor group at p-position of NBA would be expected to have a significant effect on molecular properties such as the ground and excited state dipol moments, electron density, HOMO energy level and molecular planarity.

Attempts to determine of bond length or bond order of molecules considered here using the AM1 method were unsuccessful while this method correctly predicts the expected twisted structure of molecules. We choose the two conformational parameters which define the molecular conformation (Fig. 1) the torsion angle (θ_N) which has been determined to be 55° in the solid[18] and 52° in the gas phase[15], θ_C which is $-10.3°$ in the solid[18] and nearly zero in the gas phase[15]. AM1 calculation results obtained for NBA and its derivatives are reported in Table 2 which contain some available experimental data.

Data collected in Table 2 clearly shows that the stronger the electron donor properties of substituent, the larger the angle θ_N while the enhanced accepting ability of substituent is accompanied by the lowering of θ_N in benzylidene ring. The present charecteristic trend is confirmed by plotting the θ_N against the Hammets σ_R constant, as is shown in Fig. 4. As can be seen from Table 2, there is opposite case for aniline ring (except for CH_3 group). For the same substituent, the values of θ_N are different for R1 and R2 positions.

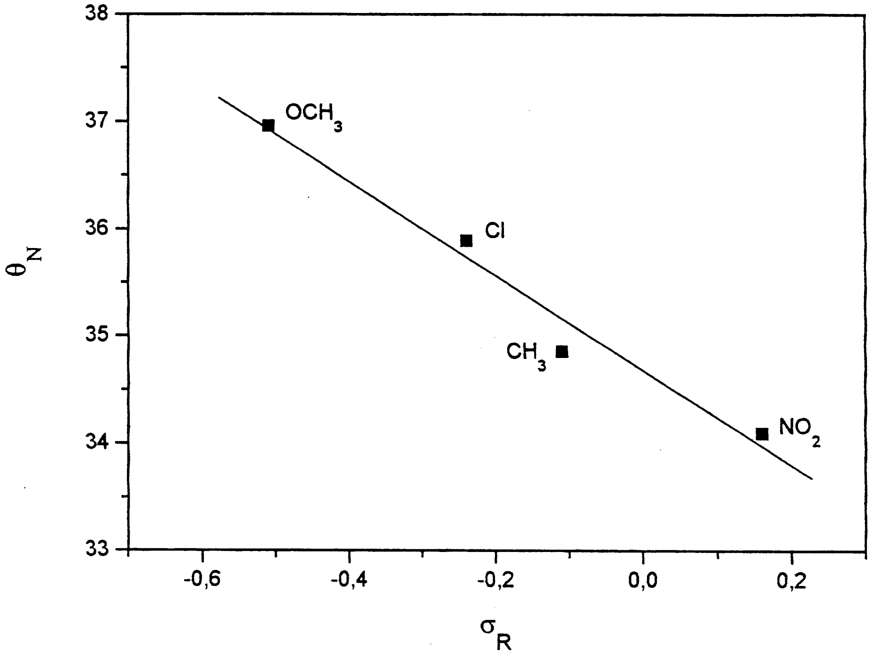

Figure 4. Plot of θ_N frequencies vs. Hammett σ_R constants in 5–8.

N-lone pair delocalization may be suppressed by the electron relasing effect of the 4-substituents resulting in less twisted conformation. In previous studies[37], explanation for the non-planarity on NBA involves a competition between two principal factors: (1) the interaction of the ortho hydrogen on the aniline ring and the hydrogen on the bridge carbon, which is repulsive in the planar conformation but is reduced with increasing non-planarity, and (2) the p-electron system: delocalization between the –CH=N- double bond and the aniline ring which is maximised for a planar conformation and delocalisation of the nitrogen lone pair electrons into the aniline ring which is essentially zero for the planar conformation but increasing non-planarity (where the lone pair density on the nitrogen may interact with the p system of the ring).

If strong electron withdrawing and electron donating groups are introduced in both ends of the molecule, the θ_N decreases to 28.38° which can be explained with increasing p-electron conjugation.

The plot of the substituent constant σ^+ against electron density at the azomethine nitrogen for benzylidene ring shows a good lineer relationship (Fig. 5). Results from Table 2 reveal that the increase of the polar structure

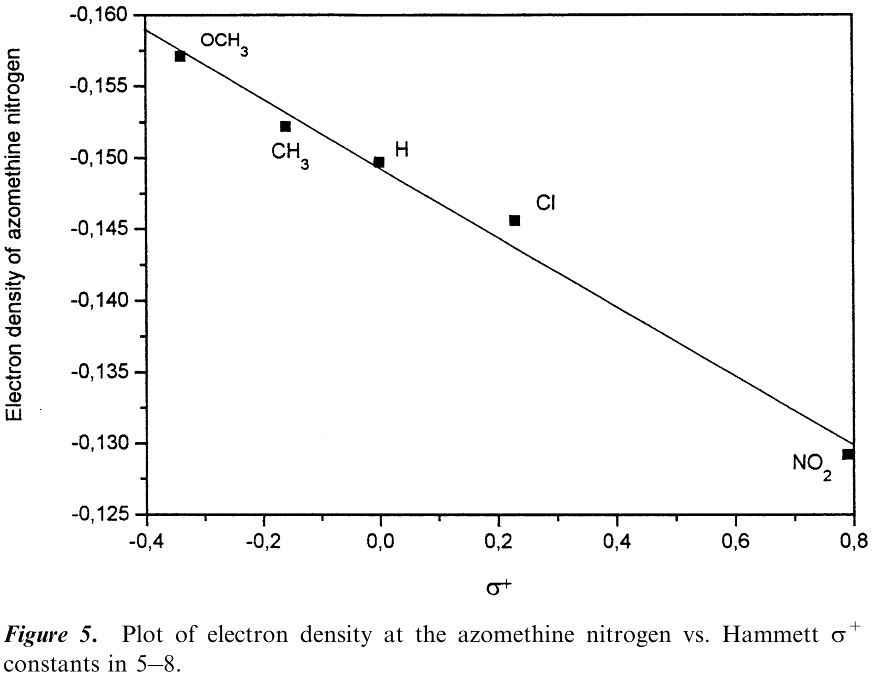

Figure 5. Plot of electron density at the azomethine nitrogen vs. Hammett σ^+ constants in 5–8.

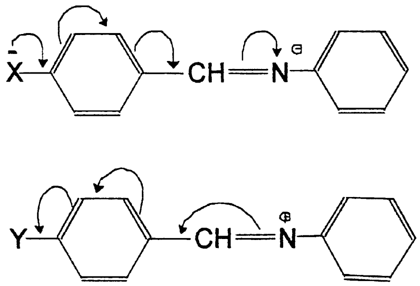

Figure 6. Substituent effect on resonance structure.

(I) to the ground state makes for an increase in the electron density of the azomethine nitrogen (Fig. 6). When substituent is an acceptor, the contribution of the polar structure (II) also increase. However, the electron density at the azomethine nitrogen decreases[4]. From these results it can be expected that C=N bond order decreases as polar structure increases. However this is not in accordance with results from AM1 MO calculation but in accordance IR results.

There is increase in the dipol moment in substutied benzylideneanilines except metoxybenzylideneaniline and benzylidenemetoxyaniline. The resonance effect of the substituents to HOMO energy levels are found significantly greater at its R1 position than that of R2 position. Electron accepting substituents lowers the HOMO energy level (Table 2).

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