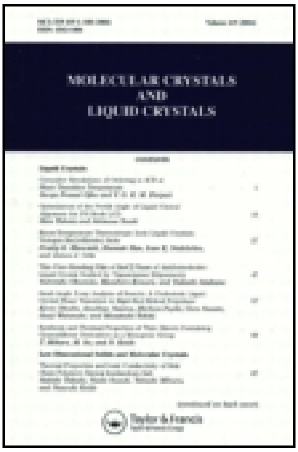

Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals

Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl19

A Study of The Possibility of Constructing A Required Crystal Structure of Nitrobenzilidene Derivatives of o-Amidoanilines by Modifying Their Molecular Structure

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To cite this article: S. M. Aldoshin , I. I. Chuev & O. A. Kozina (1995): A Study of The Possibility of Constructing A Required Crystal Structure of Nitrobenzilidene Derivatives of o-Amidoanilines by Modifying Their Molecular Structure, Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals, 264:1, 215-226

To link to this article: http://dx.doi.org/10.1080/10587259508037315

Mol. Cryst. Liq. Cryst., 1995, Vol. 264, pp. 215–226
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A Study of The Possibility of Constructing A Required Crystal Structure of Nitrobenzilidene Derivatives of *o*-Amidoanilines by Modifying Their Molecular Structure

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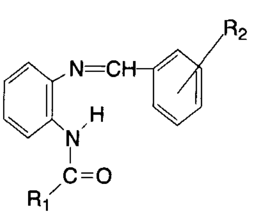
(Received September 9, 1993; in final form February 14, 1994)

An X-ray study of nitrobenzilidene derivatives of *o*-amidoanilines has been carried out. By analysis of the crystallochemical data taking into account an orienting influence of dipole–dipole interactions a relationship between the molecular and crystal structure of the compounds has been established.

INTRODUCTION

Investigations of prototropic photochemical conversions in organic crystals [1–11] demonstrate that the main conditions for proton transfer in crystal are represented by presence of intra- or intermolecular hydrogen bonds and specific character of crystal packing accounting for the proton transfer and stabilization of products. Hence an important part of the study of photochemical conversions in the crystal phase is the creation of favourable reaction conditions for a proton transfer, in particular, the study of hydrogen bond formation in a crystal.

Considering a possibility of creating potentially prototropic systems based on a new class of nitrobenzilidene derivatives of *o*-amidoanilines I–III an interesting dependence of the character of crystal packing on the peculiarities of the molecular structure of these compounds has been established. The current paper reports the results of crystallochemical analysis of a number of compounds of this class: *o*-benzamido-



I R_1 = Ph; R_2 o-NO_2
II R_1 = p—NO_2—C_6H_4
R_2 = o-NO_2
III R_1 = Ad; R_2 = m-NO_2

N-(*o*-nitrobenzilidene) aniline I, *o*-(*p*-nitrobenzamido)-*N*-(*o*-nitrobenzilidene) aniline II, *o*-(adamantanecarbamido)-*N*-(*m*-nitrobenzilidene) aniline III.

EXPERIMENTAL

Compounds I–III crystallize as yellow orthorhombic needles. The main crystal data are listed in the Table:

Compound	Space group	Z	a, Å	b, Å	c, Å	d,g/cm^3
I	$P2_12_12_1$	4	18.007(15)	18.287(13)	5.055(3)	1.377
II	Pbac	8	39.060(17)	14.026(14)	6.571(9)	1.448
III	$Pna2_1$	4	13.104(4)	22.630(11)	6.780(2)	1.341

A set of experimental reflections was obtained on a RED difractometer, CuK$_\alpha$-radiation. The data are given in the Table:

Compound	Number Ref. $I > 3\sigma$	Dimension of crystal, mm^3	*R*-factor
I	934	.5*.03*.04	0.082
II	1421	.4*.04*.05	0.047
III	1220	.6*.03*.05	0.049

The structures were solved by the direct method by the "Rentgen-75" program complex and refined by the full-matrix least-square method in anisotropic approximation. Hydrogen atoms were found from the difference Fourier synthesis and only positional parameters were refined for them. The atomic coordinates for compounds I–III are given in Tables 1–3, respectively.

Calculation of the energy of intermolecular interactions was made in the framework of atom-atomic approximations using "6-exp" potentials with parameters given in Ref. 12. Coulomb energy component was calculated from the charges obtained by the MNDO method [13]. The energy of hydrogen bond was calculated from E. M. Popov's potential:

$$U_H(d)\,\varepsilon_0^*\{1-\exp[-n(d-d_0)]\}-\varepsilon_0$$

RESULTS AND DISCUSSION

1. Molecular and Crystal Structure of I

A general view of a molecule I is given in Figure 1. The molecule is nonplanar due to large torsion angles in the amide fragment about the C^1—C^2 and N^1—C^8 bonds by 21.8° and 39.5° as well as in the azomethine fragment—about the N^2—C^{13} and C^{14}—C^{13} and C^{14}—C^{15} bonds 24.3° and 16.6° in opposite directions, respectively. In

TABLE I

Coordinates of Non Hydrogen Atoms (*10^4) and Hydrogen Atoms (*10^3) in Molecule I

Atom	X	Y	Z
O^1	2362(2)	863(3)	190(9)
O^2	3075(4)	4648(4)	3932(2)
O^3	3414(4)	4214(3)	139(2)
N^1	2558(3)	1218(2)	4121(1)
N^2	2804(3)	2463(3)	6796(1)
N^3	3011(4)	4222(3)	2087(2)
C^1	2161(3)	920(3)	2083(1)
C^2	1391(3)	666(3)	2970(1)
C^3	1049(4)	134(3)	1319(1)
C^4	356(4)	115(4)	1750(2)
C^5	38(4)	166(4)	3858(2)
C^6	267(4)	694(4)	5418(2)
C^7	988(4)	947(3)	5000(2)
C^8	3245(3)	1600(3)	3639(1)
C^9	3765(3)	1357(3)	1747(1)
C^{10}	4422(4)	1757(3)	1462(1)
C^{11}	4556(4)	2394(3)	2877(1)
C^{12}	4041(3)	2614(3)	4693(1)
C^{13}	3381(3)	2225(3)	5063(1)
C^{14}	2936(3)	2882(4)	8721(2)
C^{15}	2331(3)	3111(3)	415(1)
C^{16}	1691(3)	2683(3)	625(1)
C^{17}	1107(4)	2848(4)	2358(1)
C^{18}	1174(4)	3453(4)	4030(2)
C^{19}	1778(4)	3889(3)	3881(2)
C^{20}	2344(3)	3706(3)	2175(1)
H^1	211(6)	124(5)	625(4)
H^3	133(6)	1(5)	13(4)
H^4	7(6)	44(5)	29(4)
H^5	58(6)	9(4)	409(4)
H^6	3(6)	88(5)	700(4)
H^7	123(6)	129(5)	611(4)
H^9	360(6)	92(5)	69(4)
H^{10}	478(6)	159(5)	8(4)
H^{11}	502(6)	274(5)	223(4)
H^{12}	408(6)	313(5)	555(4)
H^{14}	340(6)	310(5)	820(4)
H^{20}	169(6)	214(5)	951(4)
H^{19}	58(6)	255(5)	281(4)
H^{18}	85(6)	351(5)	533(4)
H^{17}	191(6)	428(5)	535(4)

spite of appreciable torsion angles in these fragments, all the three phenyl rings are almost coplanar. The angle between the central phenyl (A) and *o*-nitrophenyl (B) rings in 1.5° and the angles between the *A* and *B* planes and the phenyl substituent plane (C) are 12.6° and 11.3°, respectively.

Attention is drawn to a significant torsion of the amide fragment of 39.5° with respect to the N^1—C^8 bond. It is evidently because of that fact that an intermolecular hydrogen bond $>C^1{=}O^1\cdots H^{1'}{-}N^{1'}$ ($O^1\cdots H^{1'}$ 1.93(1) Å, $O^1\cdots N^{1'}$ 2.969(6) Å, $O^1H^{1'}N^{1'}$ 155(1)°, $C^1O^1H^{1'}$ 151(1)°) has become possible in the structure between the translationally related molecules along the short "*c*" axis.

TABLE II

Coordinates of Non Hydrogen Atoms (*10^4) and Hydrogen Atoms (*10^3) in Molecule II

Atom	X	Y	Z
O^1	5647(0)	3173(2)	−5486(4)
O^2	4250(1)	4383(2)	340(4)
O^3	4508(1)	3837(2)	2978(4)
O^4	7365(0)	4213(2)	2499(4)
O^5	7473(1)	5582(2)	3864(4)
N^1	5992(0)	3314(2)	2715(3)
N^2	6520(0)	3713(1)	394(3)
N^3	4497(1)	4030(2)	1166(4)
N^4	7275(1)	4944(2)	3319(4)
C^1	5686(1)	3334(2)	3667(5)
C^2	5385(1)	3354(2)	2310(4)
C^3	5098(1)	3952(2)	3219(4)
C^4	4805(1)	4101(2)	2078(4)
C^5	4806(1)	3858(2)	44(4)
C^6	5087(1)	3459(2)	866(4)
C^7	5981(1)	3314(2)	270(4)
C^8	6316(1)	3036(2)	3511(4)
C^9	6359(1)	2569(2)	5349(4)
C^{10}	6685(1)	2297(2)	5920(5)
C^{11}	6965(1)	2476(2)	4690(5)
C^{12}	6919(1)	2950(2)	2853(5)
C^{13}	6595(1)	3247(2)	2256(4)
C^{14}	6742(1)	4243(2)	456(4)
C^{15}	6664(1)	4732(2)	2401(4)
C^{16}	6911(1)	5089(2)	3728(4)
C^{17}	6832(1)	5577(2)	5496(4)
C^{18}	6493(1)	5725(2)	5968(4)
C^{19}	6242(1)	5377(2)	4682(5)
C^{20}	6325(1)	4897(2)	2939(5)
H^1	600(6)	352(2)	148(4)
H^7	558(6)	298(2)	29(4)
H^6	508(6)	330(2)	225(4)
H^4	461(6)	444(2)	279(4)
H^3	510(6)	409(2)	471(4)
H^9	614(6)	238(2)	629(4)
H^{10}	673(6)	197(2)	722(4)
H^{11}	718(6)	222(2)	518(4)
H^{12}	712(6)	306(2)	198(4)
H^{14}	697(6)	436(2)	166(4)
H^{20}	102(6)	582(2)	627(4)
H^{19}	643(6)	602(2)	728(4)
H^{18}	600(6)	544(2)	502(4)
H^{17}	616(6)	467(2)	197(4)

The bond length in the amide fragment, within experimental error, are in the range of analogous bond length [1–10]: C^1—N^1 1.376(7) Å (1.347 1.384 Å), C^1=O^1 1.215(5) Å (1.212, 1.241 Å), demonstrating a weakened amide conjugation as a result of forming an intermolecular hydrogen bond.

The crystal packing of the molecules I (Figure 2) is characterized by "head-to-head" stacking of the benzilidenaniline fragments of translationally related molecules along the short crystallographic "*c*" axis. As has been mentioned above, the benzamide

TABLE III

Coordinates of Non Hydrogen Atoms (*10^4) and Hydrogen Atoms (*10^3) in Molecule III

Atom	X	Y	Z
O^1	1161(1)	3058(1)	7932(0)
O^2	3303(2)	5989(1)	7975(14)
O^3	3438(2)	6918(1)	8115(19)
N^1	745(2)	4026(1)	7950(9)
N^2	− 164(2)	5065(1)	7950(9)
N^3	2936(2)	6479(1)	8011(13)
C^1	1422(2)	3573(1)	8029(14)
C^2	− 490(2)	5583(1)	7986(12)
C^3	− 332(2)	4013(1)	8024(10)
C^4	− 903(2)	3494(1)	7975(10)
C^5	− 1951(2)	3529(1)	7998(13)
C^6	− 2445(2)	4067(1)	8031(12)
C^7	− 1884(2)	4583(1)	7973(14)
C^8	− 821(2)	4565(1)	7956(11)
C^9	177(2)	6103(1)	7970(11)
C^{10}	− 246(2)	6663(1)	7947(13)
C^{11}	364(2)	7158(1)	7955(14)
C^{12}	1410(2)	7107(1)	7994(14)
C^{13}	1821(2)	6542(1)	7972(11)
C^{14}	1228(2)	6040(1)	7875(10)
C^{15}	2547(2)	3751(1)	8017(12)
C^{16}	2753(2)	4416(1)	7878(16)
C^{17}	3935(2)	4529(1)	8064(18)
C^{18}	4386(6)	4246(5)	9852(15)
C^{19}	4242(7)	3624(3)	9826(16)
C^{20}	3076(5)	3489(2)	9780(12)
C^{21}	4341(7)	4279(5)	6233(14)
C^{22}	4199(5)	3573(5)	6235(16)
C^{23}	2991(6)	3489(5)	6112(14)
C^{24}	4667(3)	3331(2)	7995(31)
H^1	92(2)	435(1)	837(6)
H^2	− 126(2)	569(1)	855(5)
H^4	− 51(2)	309(1)	836(6)
H^5	− 241(2)	318(1)	808(9)
H^6	− 315(2)	410(1)	828(7)
H^7	− 221(2)	499(1)	773(8)
H^{10}	− 99(2)	674(1)	828(6)
H^{11}	2(2)	757(1)	811(9)
H^{12}	191(2)	748(1)	747(6)
H^{14}	161(2)	562(1)	784(9)
$H^{15.1}$	250(3)	472(2)	1187(6)
$H^{16.2}$	236(3)	450(2)	652(6)
H^{17}	403(2)	499(1)	768(7)
$H^{18.1}$	536(3)	436(2)	993(7)
$H^{18.2}$	434(3)	460(2)	1107(6)
H^{19}	438(3)	384(2)	1186(6)
$H^{20.1}$	267(3)	384(2)	1121(6)
$H^{20.2}$	320(3)	308(1)	866(7)
$H^{21.1}$	389(3)	439(2)	496(6)
$H^{21.2}$	506(3)	426(2)	621(7)
H^{22}	441(3)	339(2)	524(6)
$H^{23.1}$	264(3)	352(2)	502(7)
$H^{23.2}$	276(3)	299(2)	623(5)
$H^{24.1}$	547(3)	340(1)	735(5)
$H^{24.2}$	453(2)	290(1)	850(5)

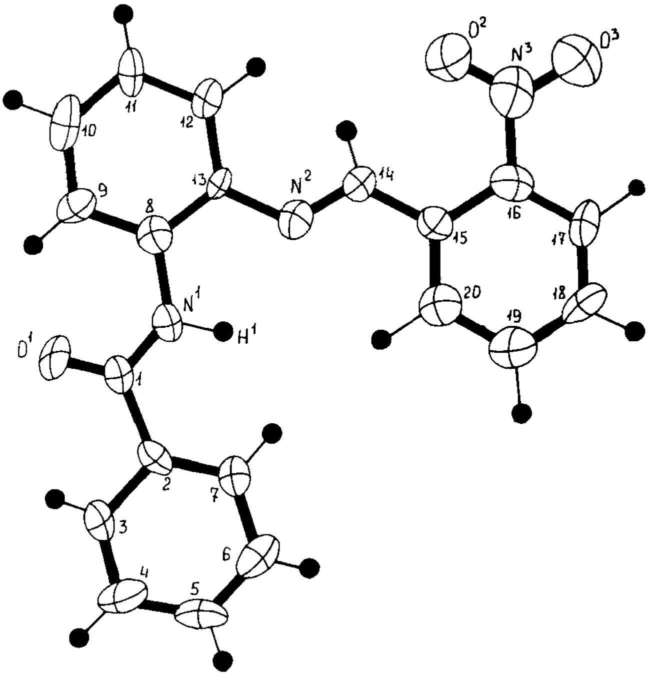


FIGURE 1 A general view of molecule I.

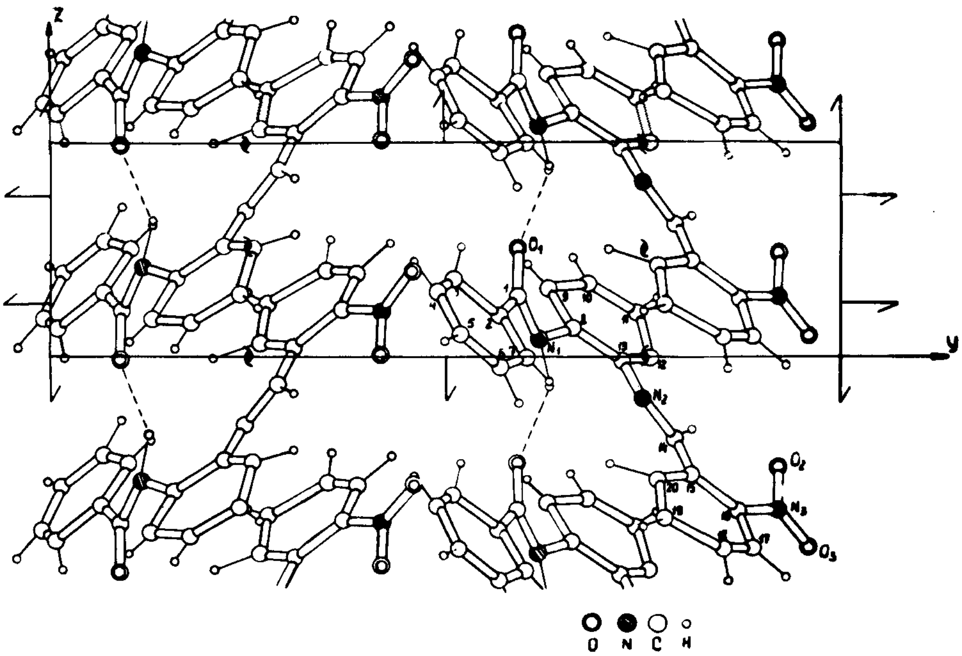


FIGURE 2 Projection of a crystal packing of molecules I on the ZYO plane.

fragments are turned from the plane of the remaining molecule part and ensure formation of intermolecular hydrogen bond along the stacks. The nonbonded contacts between the non-hydrogen atoms in the stack are in the range 3.35, 3.60 Å.

The energy of pair intermolecular interaction (IMIE) in the stacks including energy of intermolecular hydrogen bond is $-18.8/-0.3$ kcal/mol and is considerably higher than the IMIE between the molecules of the neighbouring stacks related with the initial molecule by screw axis 2_1 ($-5.9/-0.1$, $-2.2/-0.1$, $-3.7/0.1$, $-2.7/-0.1$, $-1.40/0.0$ kcal/mol). The denominator gives the Coulomb component of the IMIE. The energy of the crystal lattice is $-38.8/-2.23$ kcal/mol.

2. Molecular and Crystal Structure of II

A general view of a molecule II is given in Figure 3. As compared to I the molecule II is considerably more nonplanar. It is confirmed by large torsion angles of the azomethine fragment about the C^{13}—N^2 and C^{14}—C^{15} bonds in II by 30.2° and 22.8° in opposite directions as compared with 24.3° and 16.6° in I. However, as in I, the angle between the central phenyl (A) and *o*-nitrophenyl (B) rings is only 7.2°, while the anglles between these rings and the phenyl ring (C) is 42.8°, 47.8°, respectively. An *o*-nitrogroup in the molecule II is much highly twisted from the ring plane (33.9°) than that in I (17.2°).

Simultaneously attention is drawn to an appreciable decrease in the torsion angle about the N^1—C^8 bond down to 12.2° in II as compared with 39.5° in I. Such a planarization of this molecule part is followed by formation of a weak intramolecular hydrogen bond N^1—$H^1 \cdots N^2$ ($H^1 \cdots N^2$ 2.17(2) Å, $N^1 \cdots N^2$ 2.631(3) Å, $N^1H^1N^2$ 113(2)°, $H^1N^2C^{13}$ 81(1)°). The amide group and central phenyl fragment becoming

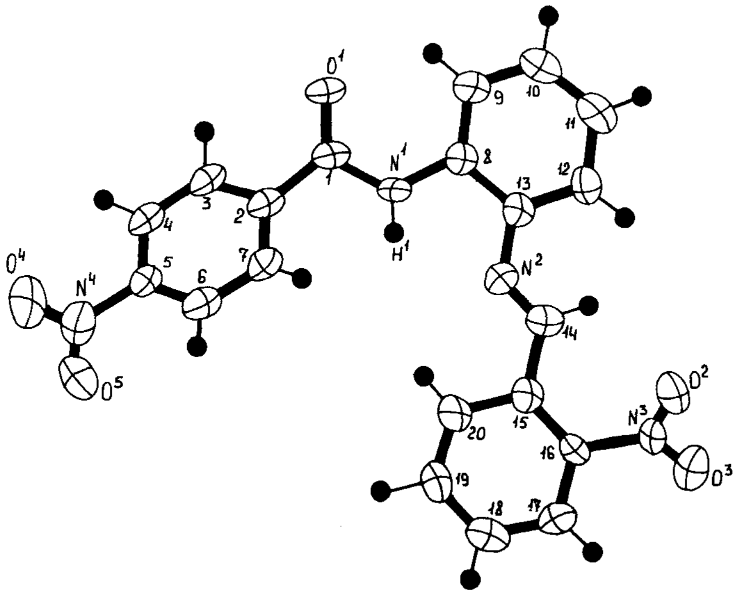


FIGURE 3 A general view of molecule II.

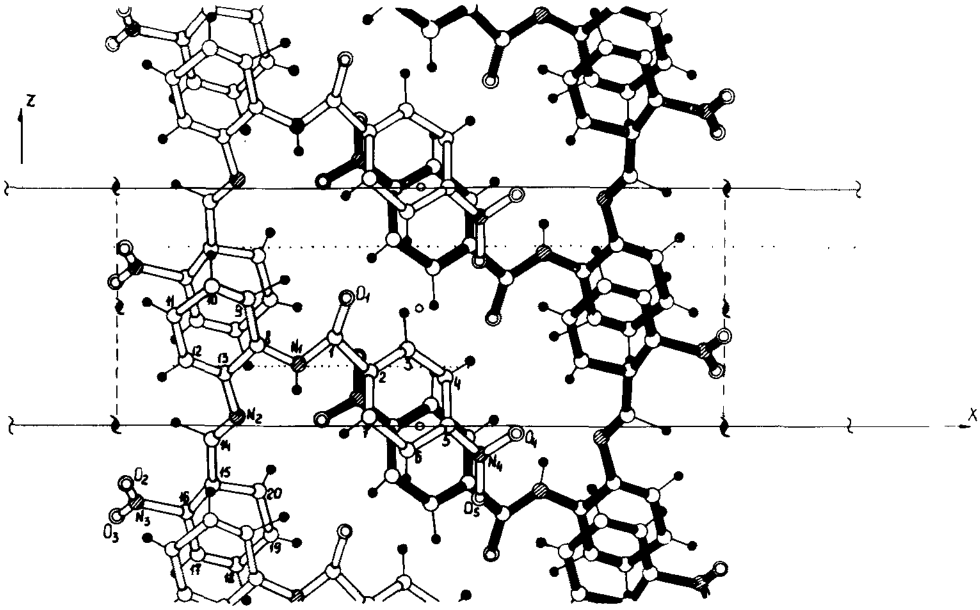


FIGURE 4 Fragment of a crystal packing of molecules II on the ZXO plane.

more planar enhances the $n_{N1}-\pi^*_{Ph}$ interaction. As a result, the N^1–C^8 bond 1.423(3) Å becomes shorter than a similar bond in the molecule I 1.442(6). The geometric modelling also shows that diminishing of the torsion angle about the N^1—C^8 bond in I would have led to a shortened intramolecular $O^1 \cdots H^9$ 1.9 Å contact, that evidently ensuring an increase in the $C^8N^1C^1$ bond angle to 128.5(3)° in II as compared with 121.5(5)° in I. The absence of intermolecular hydrogen bond and changes in the molecular geometry account for an increased basicity of the N^1 lone elctron pair (LEP) and strengthened amide conjugation revealing itself in shortening of the C^1—N^1 bond to 1.352(3) Å and lengthening of the $C^1{=}O^1$ bond to 1.226(3) Å in II as compared with 1.376(7) Å and 1.215(7) Å in I, respectively. The distribution of bond length in the azomethine fragments of both the molecules is the same within the experimental error.

A *p*-nitrogroup introduced into the benzamide fragment leads to a qualitative change in the crystal packing (Figure 4) as compared to I. As in the crystals of I, the structure of II has translational stacks along the short "*c*" axis. No intermolecular hydrogen bond in such stacks are formed since the amide groups in II are but only slightly turned about the N^1—C^8 bond from the mean plane of the benzilidenaniline fragment. The intermolecular $O^1 \cdots H^{1'}$ distance is 3.19 Å. The characteristic feature of the crystal structure II is represented by strong interstack "head-to-tail" overlapping of the *p*-nitrophenyl fragments in the "*aOc*" plane.

The IMIE in the stack (−10.9/0.0 kcal/mol) for II is less than the similar IMIE for I (−18.8/−0.3 kcal/mol) but regarding rather a strong interstack interaction (−10.9/−0.7 kcal/mol) such a packing appears to be energetically favourable, which is

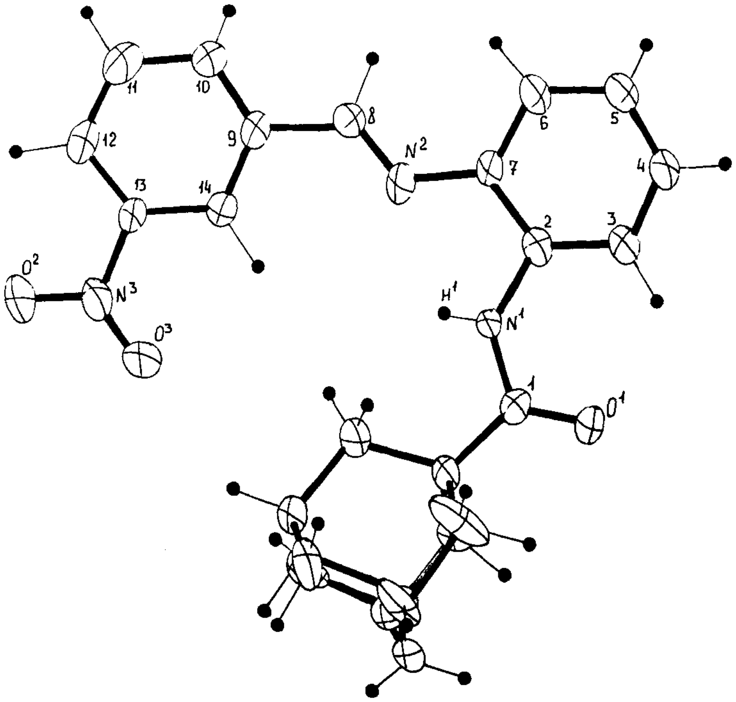


FIGURE 5 A general view of molecule III.

confirmed by the crystal lattice energy of − 37.6/− 2.6 kcal/mol close to an analogous value of − 38.8/− 2.23 kcal/mol for I.

3. Molecular and Crystal Structure of III

A general view of molecule III is given in Figure 5. The main part of the molecule excluding the adamantyl substituent is practically planar. Like in the molecule II, the orientation of the N^2 LEP and the amide H^1 atom points to formation of a week $N^1-H^1\cdots N^2$ intramolecular hydrogen bond ($H^1\cdots N^2$ 2.18(3) Å, $N^1\cdots N^2$ 2.636(2) Å, $C^7N^2H^1$ 79(1)°, $N^2H^1N^1$ 116(1)°). Diminution of the torsion angle about the $C^2—N^1$ bond (1.6°) as compared to I and II ensures further strengthening of the $n_{N}1-\pi^{*}_{Ph}$ interaction in the series I–III, the $C^1N^1C^1$ bond angle of 129.5(3)° reaching the maximum value for these compounds. The length of the $C^1—N^1$ amide bond (1.357(3) Å), within the experimental error, coincides with the similar bond length in II (1.352(3) Å).

An interesting feature of the given molecular structure is that the configuration of the N^1 atom is slightly pyramidal as compared to planar-trigonal coordination in I and II. The sum of the bond angles by the N^1 atom is 345(1)°; it lies 0.15 Å out of the coordination plane.

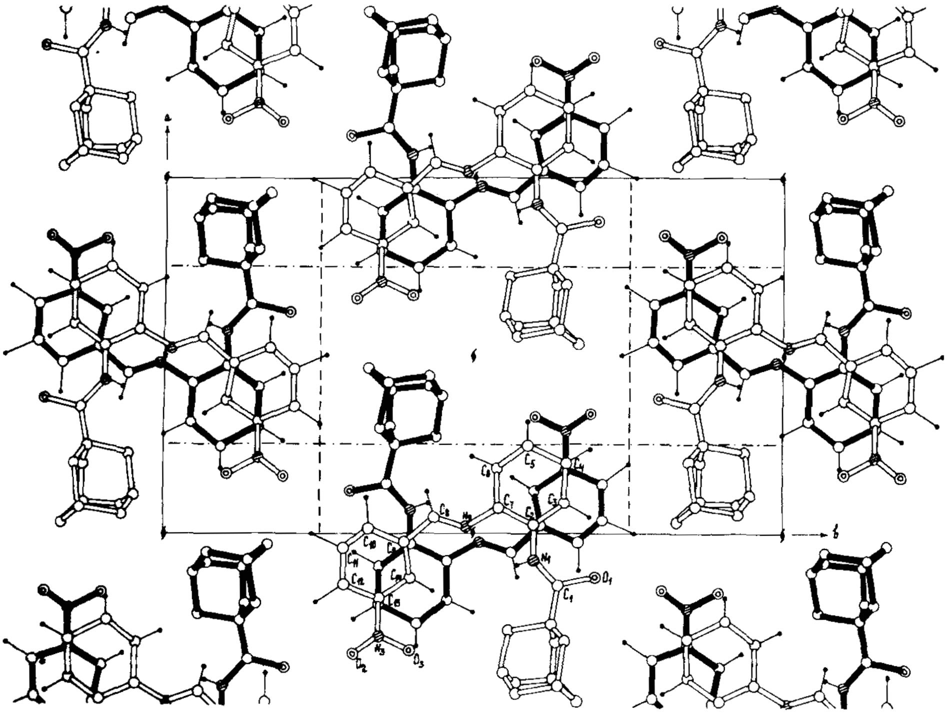


FIGURE 6 Projection of a crystal packing of molecules III on the XYO plane.

There also occurs a certain shortening of the $C^8—N^2$ bond to 1.248(3) Å as compared with 1.261(8) Å in I and 1.270(3) Å in II. It is probably connected with a decreased conjugation in the benzilidene fragment as the nitrogroup in the meta-position possesses the least acceptor abilities [14].

The crystal structure of II (Figure 6) is characterized by stacking of molecules related by a screw axis 2_1 along the short "*c*" axis. The benzilidenaniline fragments are "head-to-tail" overlapped, the adamantanecarbamide fragments of the neighbouring molecules in the stack are oppositely directed and cannot form any intermolecular hydrogen bond. The shortest contacts in the stack are in the range 3.38, 3.64 Å.

IMIE in the stack reaches −19.3/−0.2 kcal/mol, which is lower than in I (−18.8/−0.3 kcal/mol) and in II (−10.9/0.0 kcal/mol). Like in the crystals I, the IMIE in the stacks exceeds appreciably the IMIE between the molecules of the neighbouring stacks (−2.5/0.0, −2.4/−0.1, −1.9/−0.1 kcal/mol). The crystal III has the lowest value of the crystal lattice energy −39.9/−1.8 kcal/mol, in the series of compounds I–III.

4. Discussion of the Interaction between Molecular and Crystal Structure of Compounds I–III

Our X-ray studies show that the compounds I–III have quite different crystal structures, although their molecular structures are very close. If there are translational stacks in the crystal structure I where the molecules are connected by intermolecular hydrogen bond, then an introduction of a *p*-nitrogroup in the benzamide fragment of the molecule would lead in the crystals II to weakening of the interaction of molecules in the stacks and strengthening of interstack interaction. Such a changing of the crystal structure leads to larger distances between the amide and carbonyl groups. An introduction of an adamantyl substituent in the smide fragment and a replacement of an *o*-nitrophenyl sustituent by a *m*-nitrophenyl one in II leads to formation of stacks in the crystal. However, as distinct from I and II, the molecules in the stacks are oriented by the "head-to-tail" principle, that leading to an unfavourable mutual arrangement of the amide and carbonyl groups of the neighbouring molecules to form intermolecular hydrogen bond.

An insignificant contribution of the Coulomb component into the energy of the crystal studied, as compared to the Van-der-Waals interactions (I $-38.8/-2.2$ kcal/mol; II $-37.6/-2.6$ kcal/mol; III $-39.9/-1.8$ kcal/mol), allows one to believe that these interactions are not determining in the formation of the crystals I–III. However, modifications in the molecular structure of I–III touch not only the shape of the molecule but rather its dipole moment. Therefore, it is assumed that the dipole–dipole interaction, in view of its long-range character ($1/r^3$) as compared to Van-der-Waals interaction ($1/r^6$), exerts an orienting effect on the molecules during crystal growth, thus leading to an observed qualitative difference in crystal packing.

Let us analyze the dipole–dipole interactions in the studied crystals I–III. The molecules III form energetically favourable ($-19.3/-0.3$ kcal/mol) "head-to-tail" stacks in the series I–III. The dipole moment of the molecule is 3.7 D and directed almost perpendicular to the *m*-nitrobenzilidene fragment. On passing to compound I the dipole moment of the molecule decreases insignificantly to 3.5 D but its direction is changed by 93°. The total dipole moment is now oriented approximately along the angle bisector whose apex is the central phenyl ring (A) and arms are the benzamide and *o*-nitrobenzilidene substituents. Modelling of molecular stacks by the "head-to-tail" type for this compound results in shorter C···O 2.7 Å contacts between the carbonyl group carbon atom and the *o*-nitrogroup oxygen atom as well as to an increase in the dipole–dipole interaction energy to -0.2 kcal/mol, whereas for the molecules forming intermolecular hydrogen bond in the translational stacks of the actual crystal I and IMIE and dipole–dipole interaction have slightly changed ($-18.8/-0.3$ kcal/mol). In II, the dipole moment is increased to 4.0 D and its vector is turned by 85° with respect to the direction in I toward the *p*-nitrobenzamide fragment that practically coincides with the dipole moment orientation in III. The similarity in the dipole moment directions do not lead to the analogous III arrangement of molecules in the stacks. It may be explained by the above mentioned intermolecular repulsion interaction between the atoms of th *o*-nitro- and carbonyl groups. The calculation of the dipole–dipole interaction energy between the translationally related molecules II in the model crystal structure I testifies for a repulsion of 0.15 kcal/mol between them. The latter might lead to lengthening of the $O^1 \cdots H^{1'}$ distance in the crystal II when formation of intermolecular hydrogen bond becomes impossible. In the actual crystal II this energy is as low as 0.04 kcal/mol. The maximal IMIE value in the stack (-10.9 kcal/mol) for the series I–III also indicates an unfavourable mode of II.

Thus, the analysis of dipole–dipole interaction in the crystal structures of this compounds point to a possible way of constructing potentially prototropic systems through modification of molecular structure.

Acknowledgment

The work was financed by the Russian Foundation of Fundamental Investigations.

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