Available online at www.sciencedirect.com
SCIENCE DIRECT
Journal of Molecular Structure 791 (2006) 137–143
Journal of MOLECULAR STRUCTURE
www.elsevier.com/locate/molstruc

Polyamines. I. Spectroscopic properties of *N*,*N*-bis-(phthalimidopropyl)-*N*-propylamine and supramolecular interactions in its crystals

Bogumił Brycki [a,*], Iwona Kowalczyk [a], Justyna Werner [a], Teresa Borowiak [b,*], Irena Wolska [b]

[a] *Laboratory of Microbiocides Chemistry, Faculty of Chemistry, Adam Mickiewicz University, Grunwaldzka 6 60-780, Poznań, Poland*
[b] *Department of Crystallography, Faculty of Chemistry, Adam Mickiewicz University, Grunwaldzka 6 60-780, Poznań, Poland*

Received 25 November 2005; received in revised form 16 January 2006; accepted 20 January 2006
Available online 3 March 2006

Abstract

A new derivative of polyamine, *N*,*N*-bis-(phthalimidopropyl)-*N*-propylamine (**1**) has been synthesized and its structure studied by X-ray diffraction, FTIR, Raman, ^{1}H and ^{13}C NMR spectroscopies. The B3LYP and DFT calculations have been carried out. The molecular structure of *N*,*N*-bis-(phthalimidopropyl)-*N*-propylamine (**1**) presents the first case of a folded conformation for this group of compounds which is stabilized by an intramolecular hydrogen bond C–H···O. Neither C–H···π, π···π or C=O···C=O interactions operate in this case. Also the supramolecular structure is stabilized by weak C–H···O and C–H···π hydrogen bonds. The optimized bond lengths as well as bond angles for **1** calculated by B3LYP/6-31G(d,p) approach are compared with the X-ray data. The screening constants for ^{13}C and ^{1}H atoms have been calculated by the GIAO/B3LYP/6-31G(d,p) approach and analyzed. Linear correlations between the experimental ^{1}H and ^{13}C chemical shifts and the computed screening constants have been obtained.
© 2006 Elsevier B.V. All rights reserved.

Keywords: *N*,*N*-bis-(phthalimidopropyl)-*N*-propylamine; X-ray diffraction; B3LYP calculations; FTIR; Raman and NMR spectra

1. Introduction

Polymethylene polyamines occur naturally in all living species and many functions of prokaryotic and eukaryotic cells have been shown to be polyamine dependent [1,2]. On the other hand, polyamine derivatives can be used as therapeutic agents. For example, *N*-alkyl analogues of biogenic polyamines exhibit strong cytotoxic activity against human tumor cell lines [3], also naphthalimide derivatives of polyamines have potential anticancer activity [4]. Some of the polyamines and their derivatives exhibit a very good antimicrobial activity [5–7].

In order to better understand the mechanism of antimicrobial activity, we synthesized a new series of *N*,*N*-bis-(aminopropyl)-*N*-alkylamines and their derivatives. These compounds were obtained as a part of our program to develop synthetic routes to novel, stable polynuclear dendritic complexes with potential biotechnical applications. In the first step of this program, we obtained *N*,*N*-bis-(phthalimidopropyl)-*N*-propylamine, a polyamine with two terminal amine groups blocked by phthalimide moiety. Hence, the detailed structural characterization of a new phthalimide derivative is worthy of consideration.

Polyamines and their derivatives in the most cases are flexible molecules; however in some examples extended conformations are observed. Crystals with phthalimide moieties have the propensity to engage in the solid state C–H···π, π···π, dipole···dipole and other supramolecular interactions, depending on the detailed nature of the proximal functional groups [8–11]. For compounds which possess tertiary amine functions located between phthalimide moieties the interactions mentioned above lead to a folded molecular conformation as observed for compounds with the CSD codes IJOKUN, REVZEX, IJOLAU [8,9,12]. For such conformation the torsion angle N(amine)–C–C–N(phthalimide) as determined by X-ray diffraction, adopts value of about 60°. Without the possibility for C–H···π and the other interactions indicated above as in IJOKOH or IJOKAT [8] whose amino functions have been quaternized, an extended conformation is observed with the torsion angle N^{+}(amine)–C–C–N(phthalimide) of about 170°. In the folded conformation also the dipole···dipole interactions play a crucial stabilizing role. This kind of interaction is characterized by a short contact between *O*=*C* (δ+)···*O* (*δ*−)=*C* dipoles [8].

* Corresponding authors. Tel.: +48 61 829 1314; fax: +48 61 865 8008.
E-mail address: iwkow@amu.edu.pl (B. Brycki).

0022-2860/$ - see front matter © 2006 Elsevier B.V. All rights reserved.
doi:10.1016/j.molstruc.2006.01.023

Table 1
Crystal data, data collection and structure refinement for **1**

Compound	**1**
Empirical formula	$C_{25}H_{27}N_3O_4$
Formula weight	433.50
T (K)	120(2)
Wavelength (Å)	0.71073
Crystal system, space group	Triclinic, $P-1$
Unit cell dimensions	
a (Å)	8.4271(5)
b (Å)	11.2414(6)
c (Å)	11.9873(7)
α (°)	76.372(5)
β (°)	85.758(5)
γ (°)	89.296(5)
Volume (Å^3)	1100.6(1)
Z, D_x (Mg/m^3)	2, 1.308
μ (mm^{-1})	0.090
F(000)	460
θ Range for data collection (°)	3.05–30.01
hkl Range	$-11 \le h \le 11$
	$-14 \le k \le 15$
	$-16 \le l \le 8$
Reflections:	
Collected	10950
Unique (R_{int})	5560 (0.024)
Observed ($I > 2\sigma(I)$)	3982
Data/restraints/parameters	5560/0/289
Goodness-of-fit on F^2	1.019
$R(F)$ ($I > 2\sigma(I)$)	0.0423
$wR(F^2)$ (all data)	0.1104
Max/min $\Delta\rho$ (e/Å^3)	0.212/−0.206

In the current paper, we present the X-ray structure as well as results on B3LYP calculations, FTIR, Raman and NMR spectroscopy of *N*,*N*-bis-(phthalimidopropyl)-*N*-propylamine (hereafter **1**). We have been aiming in recognizing the conformational preferences of **1** whose tertiary amine function is located across longer propylene chains. Potentially, all the conditions exist to stabilize the same kind of folded conformation as in the case of compounds quoted above. However, in those examples the chains between $N_{phthalimide}$ and N_{amine} are shorter.

2. Experimental

2.1. Synthesis

N,*N*-bis-(phthalimidopropyl)-*N*-propylamine (**1**) was prepared according to the method reported previously [13]. A mixture *N*,*N*-bis-(3-aminopropyl)-amine (0.14 M) with phthalic anhydride (0.31 M) were added to ice acetic acid (300 cm^3) and stirred at room temperature for 2 h. At the next stage, *N*,*N*-bis-(phthalimidopropyl)-amine was refluxed with propylbromide (0.15 M) and sodium carbonate in ethanol for 18 h. The crude product was recrystallized from anhydrous ethanol; m.p. 109–111 °C, Yield 78%. Analysis: exp. and (calc.): %C 69.20 (69.22); %H 6.31 (6.28); %N 9.71 (9.73).

2.2. Instrumentation

Crystals suitable for X-ray analysis were grown by slow evaporation from anhydrous ethanol solution. All details of the measurements, crystal data and structure refinement are given in Table 1. The data were collected on an Oxford Diffraction KM4CCD diffractometer [14] at 120 K, using graphite-monochromated Mo K_α radiation. A total of 782 frames were measured in six separate runs. The ω-scan was used with a step of 0.75°, two reference frames were measured after every 50 frames, they did not show any systematic changes either in

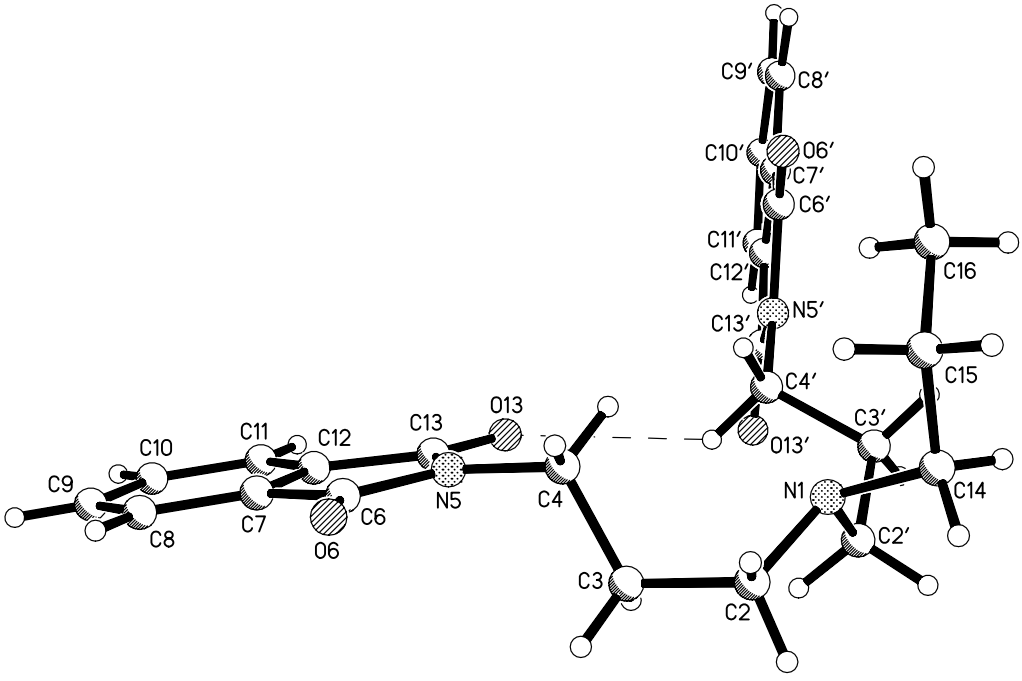

Fig. 1. A perspective view of the molecular conformation of **1** together with the atom numbering scheme.

Table 2
Hydrogen-bonding geometry (Å and deg) for **1**

D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	<(DHA)
C4′–H4′1···O13	0.97	2.60	3.300(2)	129
C8′–H8′···O13^{i}	0.93	2.53	3.461(2)	178
C10′–H10′···O13^{ii}	0.93	2.55	3.241(2)	132
C15–H15B···O6^{iii}	0.97	2.55	3.404(2)	147
C10′–H10′···O6^{iv}	0.93	2.59	3.133(2)	118
C14–H14A···*Cg*^{v}	0.97	2.78	3.570(2)	139

Cg represents the centroid of six-membered ring C7′/C8′/C9′/C10′/C11′/C12′
Symmetry codes: (i) $x-1, y, z$; (ii) $-x, -y+1, -z$; (iii) $-x+1, -y, -z-1$; (iv) $x-1, y, z+1$; (v) $-x, -y, -z$.

peak positions or in their intensities. The unit cell parameters were determined by least-squares treatment of setting angles of 5837 highest-intensity reflections chosen from the whole experiment. Intensity data were corrected for the Lorentz and polarization effects [15]. The structure was solved by direct methods with the SHELXS 97 program [16] and refined by the full-matrix least-squares method with the SHELXL 97 program [17]. The function $\sum w(|F_o|^2-|F_c|^2)^2$ was minimized with $w^{-1}=[\sigma^2(F_o)^2+(0.0605P)^2]$, where $P=(F_o^2+2F_c^2)/3$. All non-hydrogen atoms were refined with anisotropic thermal parameters. The coordinates of the hydrogen atoms were calculated in idealized positions and refined as a riding model with their thermal parameters calculated as 1.2 (1.5 for methyl group) times U_{eq} of the respective carrier carbon atom.

The NMR spectra were recorded in $CDCl_3$ on a Varian Gemini 300VT spectrometer, operating at 300.07 and 75.46 MHz for ^1H and ^{13}C, respectively.

The FTIR spectra were recorded in Nujol and Fluorolube emulsion at 2 cm^{-1} resolution on a Bruker IFS 113v spectrometer, which was evacuated to avoid water and CO_2 absorption. Raman spectra were recorded on a Nicolet Magna 760 spectrometer operating at the 1064 nm exciting line of an Nd;YAG laser. Each spectrum consists of 250 scans at 31 °C.

The calculations were performed using the GAUSSIAN 98 package [18] at the B3LYP [19,20] levels of theory with the 6-31G(d,p) basis set [21]. The molecular parameters were optimized in ab initio calculations at density-functional (DFT)

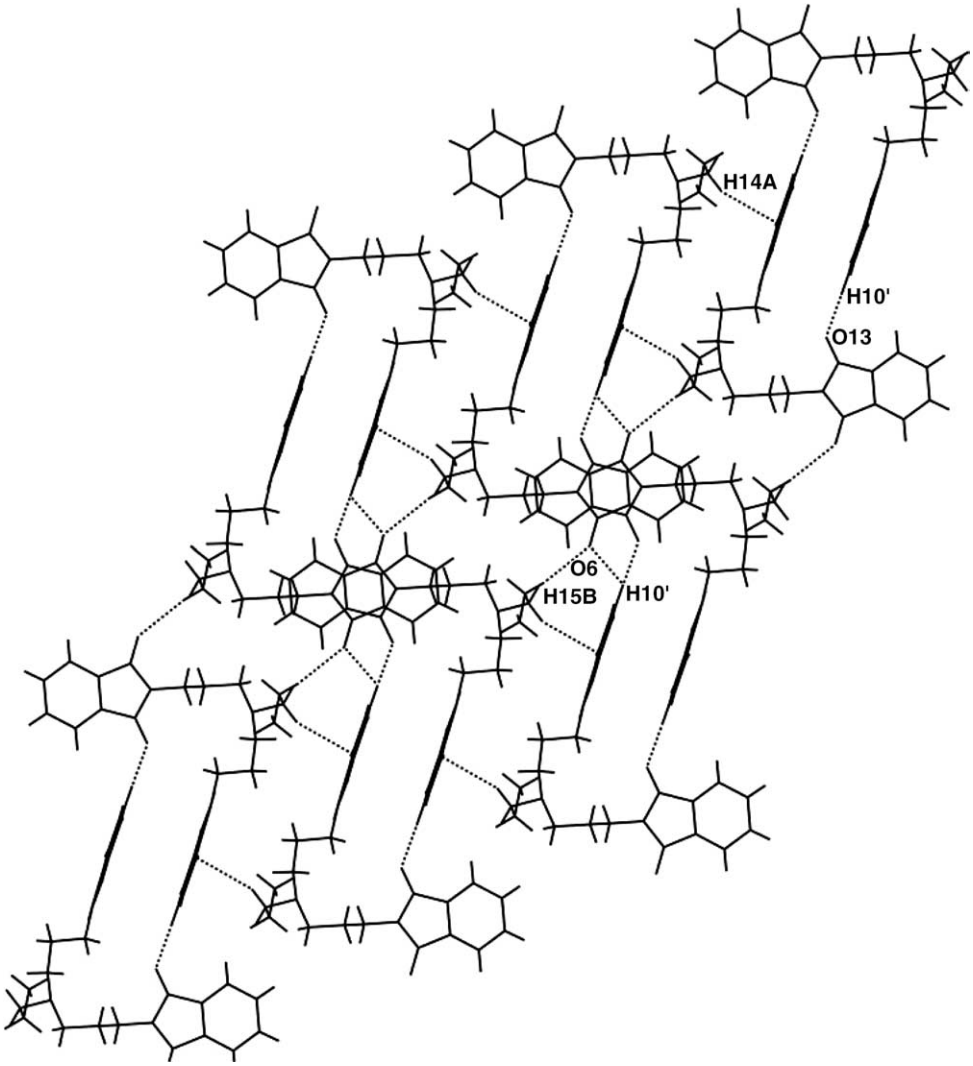

Fig. 2. The structure of one molecular sheet: centrosymmetric dimers form molecular tapes which are connected into sheets. Two tapes have been shown. Hydrogen bonds have been indicated by dashed lines.

levels of the theory using the split-valence polarized 6-31G(d,p) basis set.

CCDC 290791 for 1 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif, or by emailing data_request@ccdc.cam.ac.uk, or by contacting The Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033.

3. Results and discussion

3.1. The crystal structure of *1*

A perspective view of the molecular conformation together with the atom numbering scheme is shown in Fig. 1.

The molecule of **1** adopts a folded conformation with an angle between its phthalimide residues of 78.1(2)°. It is stabilized by the weak intramolecular hydrogen bond C(4′)–H(4′)···O(13) (Table 2) and there are no indications for the other kind of intramolecular interactions as C=O···C=O electrostatic interactions, C–H–π or π–π interactions [8]. The reason for that lies in the propyl groups which cause that the distances between the amine function and phthalimide parts as well as the both phthalimide moieties are too long. The weak hydrogen bond C–H···O is apparently competitive to the C=O···C=O electrostatic interactions for steric reasons. It is worthy of mention that the attractive interaction energies for the perpendicular motif of the C=O dipoles are comparable in strength to a C–H···O hydrogen bond [22].

Interatomic distances and angles within the phthalimide residues are normal [9]. Looking at the torsion angles in the aliphatic part of the molecule, one finds four gauche and two antibonds, although some of them are highly distorted from the ideal values. The ranges for the gauche–torsion angles are from about −63 to −86°, whereas these for antibonds are equal to about 150 and 179°. Such a broad spread is probably caused certain tension in the molecule which is caused off by the intramolecular C–H···O hydrogen bond. The packing forces influence on the conformation should be also considered (see Section 3.2.).

The supramolecular structure of **1** is unique. The molecules are organized into three-dimensional network by weak intermolecular interactions. Thus, within the crystal, centrosymmetric molecular dimers are formed *via* a pair of hydrogen bonds C10′–H10′···O13 (Table 2, Fig. 2).

The dimers are further linked via very weak C–H···π hydrogen bonds (C14–H14A···*Cg* where *g* is the centroid of a six-membered ring C7′/C8′/C9′/C10′/C11/C12′) thus forming infinite tapes along [010] axis. The tapes in turn, form two-dimensional sheets by hydrogen bonds C15–H15B···O6 and C10′–H10′···O6 (Fig. 2, Table 2). Three-dimensional supramolecular structure results from combination of sheets via hydrogen bonds C8′–H8′···O13 (Fig. 3). Surprisingly, neither

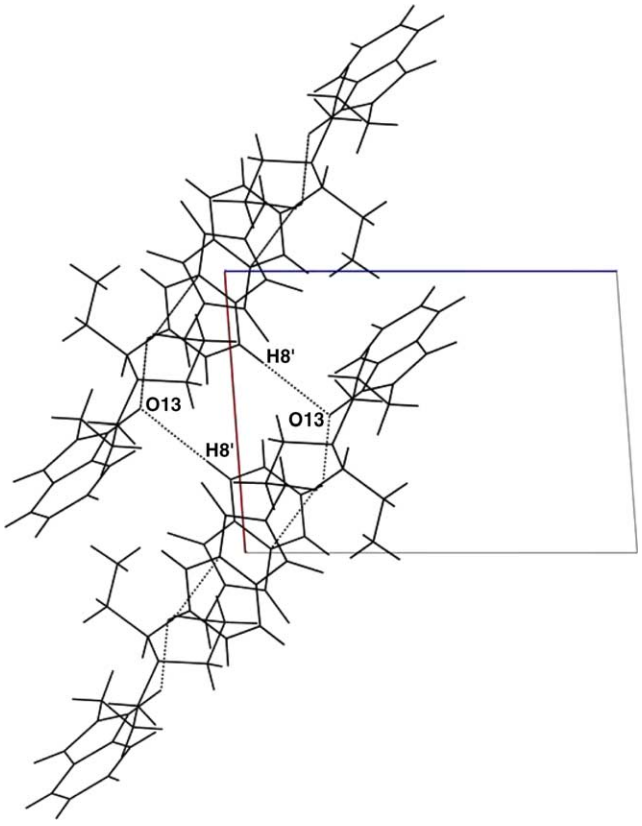

Fig. 3. The supramolecular three-dimensional structure of **1**. Molecular sheets are connected by C–H···O hydrogen bonds (dashed lines).

Table 3
Selected X-ray and B3LYP parameters of *N*,*N*-bis-(phthalimidopropyl)-*N*-propylamine (**1**)

Parameters	X-ray	B3LYP 6-31G(d,p)
Bond lengths		
N(1)–C(2)	1.471(1)	1.461
N(1)–C(14)	1.478(2)	1.468
C(4)–N(5)	1.457(2)	1.464
N(5)–C(6)	1.395(1)	1.405
N(5′)–C(6′)	1.399(2)	1.420
N(5)–C(13)	1.394(2)	1.405
N(5′)–C(13′)	1.397(2)	1.420
C(6)–O(6)	1.210(1)	1.215
C(13)–O(13)	1.212(1)	1.216
Bond angles		
C(2′)–N(1)–C(2)	111.6(1)	114.1
C(2)–N(1)–C(14)	110.1(1)	115.0
C(13)–N(5)–C(4)	123.9(1)	124.5
C(6)–N(5)–C(4)	124.3(1)	124.6
N(5)–C(6)–C(7)	106.1(1)	106.7
O(13)–C(13)–N(5)	124.8(1)	125.1
Torsion angles		
C(2′)–N(1)–C(2)–C(3)	−75.1(1)	43.9
C(14)–N(1)–C(2)–C(3)	160.7(1)	−91.8
C(2)–C(3)–C(4)–N(5)	179.3(1)	68.6
C(3)–C(4)–N(5)–C(13)	−83.0(1)	60.8
C(3)–C(4)–N(5)–C(6)	93.1(1)	−122.5
C(13)–N(5)–C(6)–O(6)	179.1(1)	178.9
O(6)–C(6)–C(7)–C(8)	−0.6(2)	0.8
N(5)–C(6)–C(7)–C(8)	179.8(1)	−179.7

Table 4
Chemical shifts (δ, ppm) in $CDCl_3$ and calculated GIAO nuclear magnetic shielding tensors (σ_{cal}) for *N*,*N*-bis-(phthalimidopropyl)-*N*-propylamine (**1**)

	$\delta_{exp.}$	$\delta_{calc.}$	$\sigma_{calc.}$		$\delta_{exp.}$	$\delta_{calc.}$	$\sigma_{calc.}$
C (2)	51.5	48.8	46.9	H (2)	2.49	2.72	2.31
C (3)	26.3	31.2	30.0	H (3)	1.80	1.91	1.59
C (4)	36.5	36.7	35.3	H (4)	3.74	3.73	3.36
C (6,13)	168.4	171.8	165.2	H (8,11)	7.81	7.83	7.57
C (7,12)	133.8	133.5	128.4	H (9,10)	7.72	7.61	7.38
C (8,11)	132.2	129.7	124.7	H (14)	2.36	2.42	2.08
C (9,10)	123.0	121.4	116.7	H (15)	1.41	1.43	1.07
C (14)	55.6	53.4	51.4	H (16)	0.88	0.75	0.36
C (15)	20.1	23.2	22.3				
C (16)	11.9	9.5	9.1				

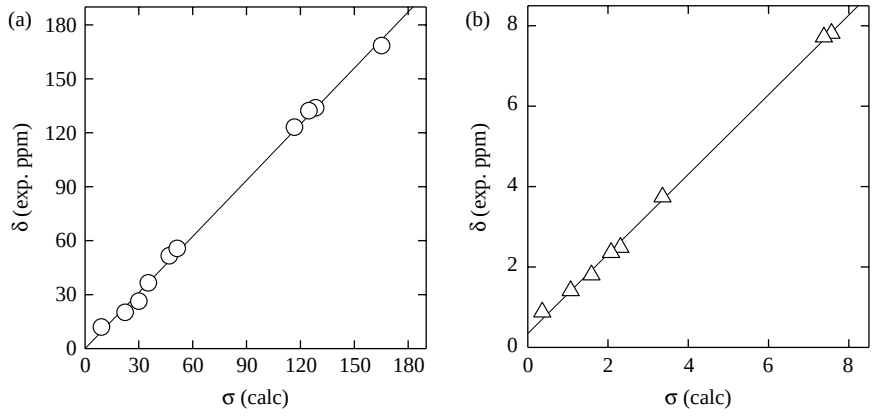

Fig. 4. The relationship (a) between the experimental ^{13}C chemical shifts (δ) and the GIAO computed ^{13}C screening constants (σ) and (b) between the experimental ^{1}H chemical shifts (δ) and the GIAO computed ^{1}H screening constants (σ).

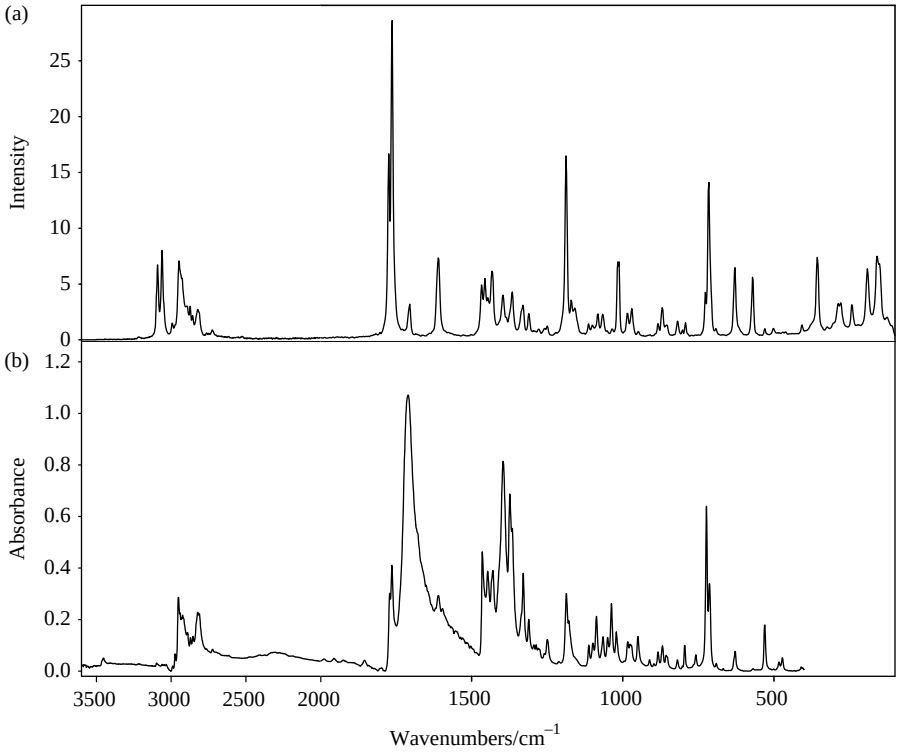

Fig. 5. The spectra of *N*,*N*-bis-(phthalimidopropyl)-*N*-propylamine: (a) Raman spectrum in the solid state; and (b) FTIR spectrum in Nujol and Fluorolube emulsion.

intermolecular interactions C=O···C=O nor π···π have been found.

3.2. B3LYP calculations

The optimized geometry parameters computed by using of the B3LYP are compared with the X-ray diffraction data in Table 3. The experimental and calculated bond lengths and bond angles are comparable in the most cases.

According to the dihedral angles presented in Table 3, the molecules in the gas-phase are more folded in comparison to those in the crystal. The conformation differences are probably caused by intermolecular interactions in crystals. It is well known that intermolecular interactions may cause the molecular geometry in the crystals to be different from that of the free molecules [23].

3.3. ^{1}H NMR and ^{13}C NMR spectra

The proton chemical shift assignments are based on the 2D COSY experiments, in which the proton–proton connectivity is observed through the off-diagonal peaks in the counter plot. The 2D heteronuclear shifts correlated counter map (HETCOR) has been used to identify resonance signals in the ^{13}C NMR spectra.

The experimental chemical shifts in $CDCl_3$ and the GIAO shielding constants calculated for **1** are listed in Table 4. The corelations between the experimental ^{1}H and ^{13}C chemical shifts (δ_{exp}) and the computed screening constants ($\sigma_{calc.}$) are shown in Fig. 4. For ^{1}H and ^{13}C the correlation is linear and described by the following equation:

$$\delta_{exp} = A\sigma_{calc} + B$$

Values of the slope ($A_C = 1.0401$, $A_H = 0.9904$) and intercept ($B_C = -6.8923$, $B_H = 0.3423$) were determined through a fit of the computed shielding constants to the experimental chemical shifts.

The very good correlation coefficients ($r^2 = 0.999$) for ^{1}H and ($r^2 = 0.998$) for ^{13}C correlations confirm the optimized geometry of **1**.

3.4. FTIR and Raman spectra

The IR and Raman spectra of **1** in the solid state are presented in Fig. 5 and the assignments proposed are given in Table 5. These assignments are partly based on the calculated spectrum of *N*-aminophthalimide [24].

In general, the bands around 1650–1350 cm^{-1} in FTIR spectra are assigned to skeletal C–C stretching modes of benzene ring. The C–N stretching vibrations of **1** are observed at 1187 and 1178 cm^{-1}.

The FTIR spectrum of **1** shows characteristic bands at 1771 and 1764 cm^{-1} which are due to asymmetric stretching vibrations of carbonyl group $\nu_{as}C{=}O$ in a phthalimide moiety [25,26]. The symmetric stretching vibration $\nu_{s}C{=}O$ appears in the FTIR spectrum as a broad and intensive band at 1710 cm^{-1}. In the Raman spectrum, this absorption is very small and lies at 1705 cm^{-1} [27]. The difference between intensities of symmetric and asymmetric stretching vibrations of carbonyl groups is connected with the symmetry of the molecule. When two C=O bonds are not coplanar the intensity of $\nu_{as}C{=}O$ should be lower than that of the $\nu_{s}C{=}O$ [24]. The split of $\nu_{as}C{=}O$ band suggests the non-equivalence of carbonyl groups in phtalimide moiety which is confirmed by X-ray data.

Table 5
FTIR and Raman frequencies of *N*,*N*-bis-(phthalimidopropyl)-*N*-propylamine (**1**)

Raman	FTIR	Proposed assignment
3091		νCH
3061	2974	νCH
2947	2952	νCH_2
2925	2924	νCH_2
2873	2871	νCH_2
2856	2854	νCH_2
2822	2822	νCH_2
1774	1771	$\nu_{as}CO$
1763	1764	$\nu_{as}CO$
1705	1710	$\nu_{s}CO$
1610	1610	νCC
1467	1465	νCC
1456	1447	$\delta_{as}CH_3$
1432	1430	νCC
1396	1396	νCC
	1374	$\delta_{as}CH_3$
1366	1366	νCC, δCH_2
1330	1329	δCH_2
1311	1311	δCH_2
	1294	νCC
	1286	νCC
1278	1279	νCC
1249	1250	δCH_2
	1212	νCC
1188	1187	νCN
1170	1178	νCN
1113	1113	βCH
1110	1099	βCH
1083	1087	γCH
1066	1065	γCH
	1050	νCC
1035	1038	δCH_2
1016	1021	βCC
985	984	γCH
970	976	γCH
949	950	δCH_2
	911	δCO
	897	γCH
883	883	βCC
869	869	γCH
856	857	νCC
819	819	νCC
792	795	γCH
	759	τring
	723	δCO
716	713	βCC
692	691	βring
629	628	γCH
531	531	γCC
	483	τring
461	472	τring

4. Conclusions

The molecular and crystal structures of *N*,*N*-bis-(phthalimidopropyl)-*N*-propylamine (**1**) have been determined by X-ray diffraction and by the B3LYP calculations. The crystal structure of **1** presents the first case of a folded conformation of *N*-alkylamine-phthalimides which is stabilized by an intramolecular hydrogen bond C–H···O. Also the supramolecular structure is stabilized by the C–H···O and C–H···π hydrogen bonds. No C=O···C=O interactions have been found.

Both FTIR and Raman spectra are consistent with the observed structure in the crystal.

Good correlations between the experimental ^{13}C and ^{1}H chemical shifts in $CDCl_3$ solution of **1** and GIAO/B3LYP/6-31G(d,p) calculated isotropic shielding tensors ($\delta_{exp} = A\sigma_{calc} + B$) have confirmed the optimized geometry of **1**.

Acknowledgements

This work was supported by the funds from Adam Mickiewicz University, Faculty of Chemistry.

References

[1] G. Karigiannis, D. Papaioannou, Eur. J. Org. Chem. (2000) 1841.
[2] H.M. Wallace, A.V. Fraser, A. Hughes, Biochemistry 376 (2003) 1.
[3] P.V. Thoo Lin, A.M. Dance, C. Bestwick, L. Milner, Biochem. Soc. Trans. 31 (2003) 407.
[4] M.F. Brana, A. Ramos, Curr. Med. Chem. (2001) 237.
[5] S.S. Block, Disinfection, Sterilization and Preservation LWW, Philadelphia, 2001.
[6] B. Brycki, J. Werner, Ann. Pol. Chem. Soc. 3 (2004) 139.
[7] B. Brycki, K. Seifert, F. Domka, Pol. J. Environ. Stud. 14 (2005) 411.
[8] R.C. Howell, S.H. Edwards, A.S. Gajadhar-Plummer, I.A. Kahwa, G.L. PcPherson, J.T. Mague, A.J.P. White, D.J. Williams, Molecules 8 (2003) 565.
[9] D.M.Y. Barrett, I.A. Kahwa, J.T. Mague, G.L. McPherson, J. Org. Chem. 60 (1995) 5946.
[10] D.M.Y. Barrett, I.A. Kahwa, D.J. Williams, Acta Crystallogr. C52 (1996) 2069.
[11] D.M.Y. Barrett, I.A. Kahwa, B. Radüchel, A.J.P. White, D.J. Williams, J. Chem. Soc. Perkin Trans. 2 (1998) 1851.
[12] F.H. Allen, Acta Crystallogr. B58 (2002) 380.
[13] B. Brycki, J. Werner, I. Kowalczyk, Pol. J. Chem, in press.
[14] Oxford Diffraction Poland, CrysAlisCCD, CCD Data Collection GUI, Version 1.171, 2003.
[15] Oxford Diffraction Poland, CrysAlisRED, CCD Data Reduction GUI, Version 1.171, 2003.
[16] G.M. Sheldrick, Acta Crystallogr. A46 (1990) 467.
[17] G. M. Sheldrick, SHELXL97, Program for the Refinement of Crystal Structures, University of Göttingen, Germany, 1997.
[18] M. J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, V.G. Zakrzewski, A.J. Jr. Montgomery, R.E. Stratmann, J.C. Burant, S. Dapprich, J.M. Millam, A.D. Daniels, K.N. Kudin, M.C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G.A. Petersson, P.Y. Ayala, Q. Cui, K. Morokuma, D.K. Malick, A.D. Rabuck, K. Raghavachari, J.B. Foresman, J. Cioslowski, J.V. Ortiz, B.B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R.L. Martin, D.J. Fox, T. Keith, M.A. Al-Laham, C.Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe, P.M.W. Gill, B. Johnson, W. Chen, M.W. Wong, J.L. Andres, C. Gonzalez, M. Head-Gordon, E.S. Replogle, J.A. Pople, GAUSSIAN 98, Revision A 6, Gaussian, Inc, Pittsburg, PA, 1998.
[19] A.D. Becke, J. Chem. Phys. 98 (1993) 5648.
[20] P.J. Stephenss, F.J. Devlin, C.F. Chabalowski, M.J. Frisch, J. Phys. Chem. 98 (1994) 11623.
[21] W.J. Hehre, L. Random, P.V.R. Schleyer, J.A. Pople, Ab Initio Molecular Orbital Theory, Wiley, New York, 1986.
[22] F.H. Allen, Ch.A. Baalham, J.P.M. Lommerse, P.R. Raithby, Acta Crystallogr. B54 (1998) 320.
[23] I. Hargittai, Pure Appl. Chem. 61 (1989) 651; J.F. Chiang, J.J. Song, J. Mol. Struct. 96 (1982) 151.
[24] N. Puvierasan, V. Arjunan, S. Mohan, Turk. J. Chem. 26 (2002) 323.
[25] I.M. Gulis, A.I. Komyak, K.A. Saechnikov, V.A. Tsvirko, J. Appl. Spectrosc. 58 (1993) 36.
[26] B.A. Poyor, P.M. Palmer, P.M. Andrews, M.B. Berger, T. Troxler, Chem. Phys. Lett. 271 (1997) 19.
[27] E. Tatsch, B. Schrader, J. Raman. Spectrosc. 26 (1995) 467.