Oxidative macrocyclocondensation of 3,4-diaminofurazan and 4,4′-diamino-3,3′-azofurazan with dibromoisocyanurate. Crystal structures of hexa- and octadiazenofurazan macrocycles

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The oxidative cyclocondensation of 3,4-diaminofurazan and 4,4′-diamino-3,3′-azofurazan with dibromoisocyanurate afforded macrocyclic polydiazenofurazans. The reaction can be directed towards the formation of both the four-membered cycle alone or the three-, six-, and eight-membered macrocycles.

Key words: diamine, dibromoisocyanurate, oxidative macrocyclocondensation; X-ray structural analysis.

Earlier[1] it has been shown that a mixture of $Pb(OAc)_4$ and Bu_4NBr reacts with 3,4-diaminofurazan (DAF) and 4,4′-diamino-3,3′-azofurazan (DAAF) to afford previously unknown macrocyclic polydiazenofurazans **1**—**5** and **1**—**3**, respectively. However, from the synthetic point of view, these methods are suitable only for the synthesis of compound **1**.

Macrocycle **1** has been also obtained[2] by the intramolecular cyclization of 4,4′-bis(4-aminofurazanyl-3-azo)-3,3′-azofurazan (**6**), which proceeds *via* treatment not only with a mixture of $Pb(OAc)_4$ and Bu_4NBr but also with dibromoisocyanurate (DBI), which earlier has been used for oxidation of heterocyclic amines to azo compounds[3] and for the synthesis of macrocycles from diamines containing amino groups at furazan cycles.[4,5]

The oxidative condensation of DAF and DAAF under the action of DBI in different solvents (MeCN, C_6H_6, CH_2Cl_2, MeOH, CH_2Cl_2—EtOAc (2 : 1), and CH_2Cl_2—MeCN (2 : 1)) has been studied in this work. It is shown that oxidation with this reagent results also in the formation of macrocycles **1**—**5**. However, the results of the reaction depend significantly on the type of a solvent, the [diamine] : [DBI] ratio, and their concentrations.

The reaction of DAAF with a 2.5—6-fold excess of DBI in MeCN affords a mixture of macrocycles **1**—**3** with an even number of diazenofurazan fragments. Under the same conditions, DAF affords a mixture of these compounds with macrocycles **4** and **5** containing an odd number of diazenofurazan fragments, with compound **1** predominating substantially in the reaction products (Scheme 1) like under the action of a mixture of $Pb(OAc)_4$ and Bu_4NBr.[1] Varying the amount of a solvent, we found both conditions that allow one to obtain tetradiazenofurazan **1** in a preparative yield (88 %) and conditions that increase the yield of macrocycles **2** and **3** (<1 %)[1] to 35 % and 8 %, respectively. It has been established that carrying out the reactions in considerably more concentrated (10—15 times) solutions than are needed for the preparation of tetradiazenofurazan **1** favors the formation of macrocycles with $n > 4$.

The reaction of DAAF with a twofold excess of DBI in MeCN or with its 1.7—3-fold excess in other solvents resulted in the formation of a linear product of the oxidative dimerization **6*** or a mixture of compounds **6** and **1** (20—40 %). Diamine **6** was isolated from a mixture with the starting compound in a 15 % yield.

We succeeded in obtaining three-membered macrocycle **4** in a higher yield (12.5 %) than before[1] when the reaction with DAF was carried out in MeOH, and DBI was added in portions. After the reaction of DAF with DBI in MeCN, compound **5** was only found in mixtures with other macrocycles.

† Deceased in 1995.

* Compound **6** was identified by comparison with a previously known sample synthesized by V. O. Kulagina (N. D. Zelinsky Institute of Organic Chemistry of the RAS) using another method.

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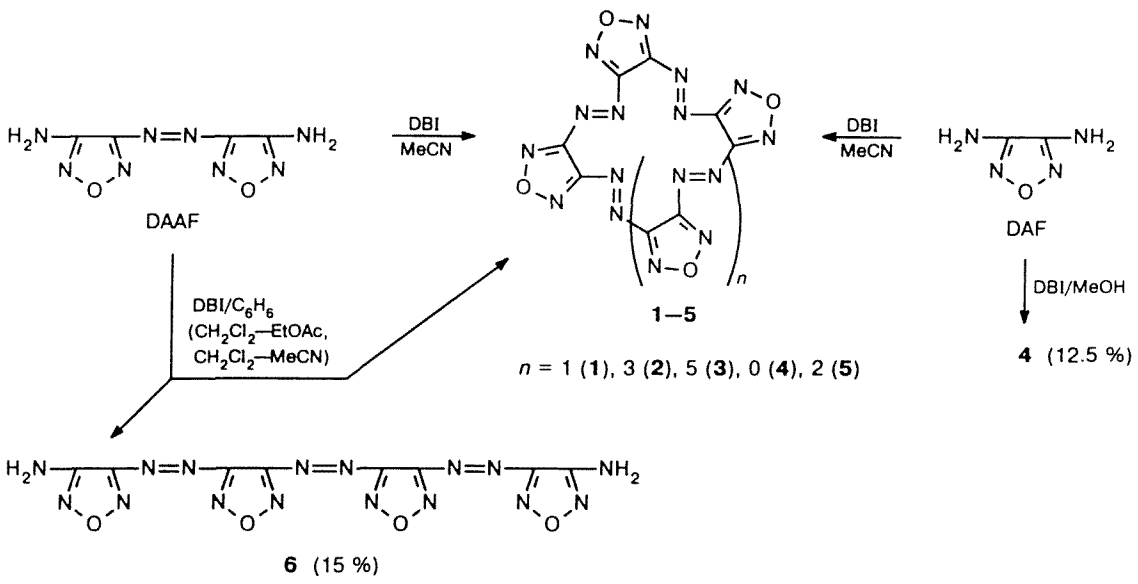
Scheme 1



The structure of compounds **2** and **3** was determined by X-ray structural analysis and compared with that of macrocycle **1** previously studied by this method.[2]

The general views of molecules **2** and **3** (molecule **2** is located on crystallographic axis *2* and molecule **3** at the center of symmetry) are shown in Figs. 1 and 2, respectively. Bond lengths are given in Table 1, bond angles are given in Table 2, and Table 3 presents the torsion and dihedral angles in structures **2** and **3**. Macrocycles **2** and **3** (24- and 32-membered, respectively) are composed of

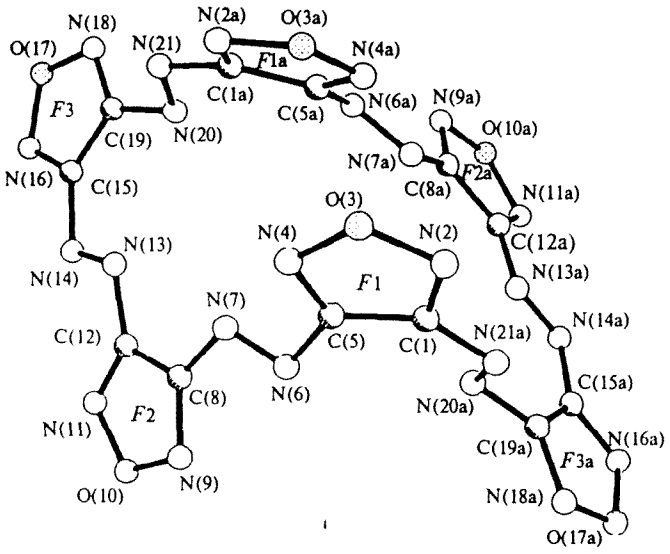


Fig. 1. Structure of molecule **2**.

Table 1. Bond lengths (*d*) in molecules **2** and **3**

Molecule 2		Molecule 3	
Bond	*d*/Å	Bond	*d*/Å
C(1)—N(2)	1.320(4)	O(1)—N(1)	1.374(3)
C(1)—C(5)	1.423(6)	O(1)—N(2)	1.353(3)
C(1)—N(21a)	1.408(5)	O(2)—N(5)	1.368(3)
N(2)—O(3)	1.367(4)	O(2)—N(6)	1.372(3)
O(3)—N(4)	1.391(4)	O(3)—N(9)	1.381(3)
N(4)—C(5)	1.316(4)	O(3)—N(10)	1.370(3)
C(5)—N(6)	1.420(5)	O(4)—N(13)	1.377(3)
N(6)—N(7)	1.257(4)	O(4)—N(14)	1.382(3)
N(7)—C(8)	1.421(5)	N(1)—C(1)	1.294(3)
C(8)—N(9)	1.309(4)	N(2)—C(2)	1.301(3)
C(8)—C(12)	1.417(4)	N(3)—N(4)	1.225(3)
N(9)—O(10)	1.386(4)	N(3)—C(2)	1.412(3)
O(10)—N(11)	1.373(3)	N(4)—C(3)	1.432(3)
N(11)—C(12)	1.311(5)	N(5)—C(3)	1.294(3)
C(12)—N(13)	1.407(4)	N(6)—C(4)	1.305(3)
N(13)—N(14)	1.258(4)	N(7)—N(8)	1.241(3)
N(14)—C(15)	1.413(4)	N(7)—C(4)	1.410(3)
C(15)—N(16)	1.303(4)	N(8)—C(5)	1.416(3)
C(15)—C(19)	1.427(6)	N(9)—C(5)	1.297(3)
N(16)—O(17)	1.367(4)	N(10)—C(6)	1.304(3)
O(17)—N(18)	1.393(4)	N(11)—N(12)	1.250(3)
N(18)—C(19)	1.285(4)	N(11)—C(6)	1.405(3)
C(19)—N(20)	1.430(4)	N(12)—C(7)	1.407(3)
N(20)—N(21)	1.267(4)	N(13)—C(7)	1.300(3)
N(21)—C(1a)	1.408(5)	N(14)—C(8)	1.290(3)
		N(15)—N(16)	1.220(3)
		N(15)—C(8)	1.418(3)
		N(16)—C(1a)	1.427(3)
		C(1)—C(2)	1.412(3)
		C(1)—N(16a)	1.427(3)
		C(3)—C(4)	1.414(3)
		C(5)—C(6)	1.423(3)
		C(7)—C(8)	1.426(3)

Table 2. Bond angles (ω) in molecules **2** and **3**

Molecule **2**		Molecule **3**	
Angle	ω/deg	Angle	ω/deg
N(2)—C(1)—C(5)	108.6(3)	N(1)—O(1)—N(2)	111.4(2)
N(2)—C(1)—N(21a)	118.0(3)	N(5)—O(2)—N(6)	112.1(2)
C(5)—C(1)—N(21a)	133.5(3)	N(9)—O(3)—N(10)	111.9(2)
C(1)—N(2)—O(3)	105.6(3)	N(13)—O(4)—N(14)	111.5(2)
N(2)—O(3)—N(4)	111.7(2)	O(1)—N(1)—C(1)	105.2(2)
O(3)—N(4)—C(5)	104.5(3)	O(1)—N(2)—C(2)	105.6(2)
C(1)—C(5)—N(4)	109.5(3)	N(4)—N(3)—C(2)	111.8(2)
C(1)—C(5)—N(6)	127.0(3)	N(3)—N(4)—C(3)	112.9(2)
N(4)—C(5)—N(6)	123.0(4)	O(2)—N(5)—C(3)	104.9(2)
C(5)—N(6)—N(7)	111.5(3)	O(2)—N(6)—C(4)	104.4(2)
N(6)—N(7)—C(8)	112.7(3)	N(8)—N(7)—C(4)	111.6(2)
N(7)—C(8)—N(9)	126.8(3)	N(7)—N(8)—C(5)	112.9(2)
N(7)—C(8)—C(12)	123.8(3)	O(3)—N(9)—C(5)	105.0(2)
N(9)—C(8)—C(12)	109.4(3)	O(3)—N(10)—C(6)	104.7(2)
C(8)—N(9)—O(10)	104.1(2)	N(12)—N(11)—C(6)	112.6(2)
N(9)—O(10)—N(11)	112.5(2)	N(11)—N(12)—C(7)	110.5(2)
O(10)—N(11)—C(12)	104.2(3)	O(4)—N(13)—C(7)	104.7(2)
C(8)—C(12)—N(11)	109.8(3)	O(4)—N(14)—C(8)	105.2(2)
C(8)—C(12)—N(13)	123.0(3)	N(16)—N(15)—C(8)	114.7(2)
N(11)—C(12)—N(13)	127.2(3)	N(15)—N(16)—C(1a)	110.4(2)
C(12)—N(13)—N(14)	113.9(3)	N(1)—C(1)—C(2)	109.0(2)
N(13)—N(14)—C(15)	109.2(3)	N(1)—C(1)—N(16a)	122.8(2)
N(14)—C(15)—N(16)	120.1(3)	C(2)—C(1)—N(16a)	128.1(2)
N(14)—C(15)—C(19)	130.8(3)	N(2)—C(2)—N(3)	116.4(2)
N(16)—C(15)—C(19)	109.1(3)	N(2)—C(2)—C(1)	108.8(2)
C(15)—N(16)—O(17)	105.2(3)	N(3)—C(2)—C(1)	134.8(2)
N(16)—O(17)—N(18)	111.2(2)	N(4)—C(3)—C(5)	126.1(2)
O(17)—N(18)—C(19)	105.2(3)	N(4)—C(3)—C(4)	124.2(2)
C(15)—C(19)—N(18)	109.3(3)	N(5)—C(3)—C(4)	109.4(2)
C(15)—C(19)—N(20)	127.2(3)	N(6)—C(4)—N(7)	118.1(2)
N(18)—C(19)—N(20)	123.0(4)	N(6)—C(4)—C(3)	109.2(2)
C(19)—N(20)—N(21)	111.9(3)	N(7)—C(4)—C(3)	132.7(2)
N(20)—N(21)—C(1a)	110.4(3)	N(8)—C(5)—N(9)	123.0(2)
		N(8)—C(5)—C(6)	127.6(2)
		N(9)—C(5)—C(6)	108.9(2)
		N(10)—C(6)—N(11)	117.5(2)
		N(10)—C(6)—C(5)	109.5(2)
		N(11)—C(6)—C(5)	133.0(2)
		N(12)—C(7)—N(13)	119.7(2)
		N(12)—C(7)—C(8)	130.9(2)
		N(13)—C(7)—C(8)	109.4(2)
		N(14)—C(8)—N(15)	125.5(2)
		N(14)—C(8)—C(7)	109.2(2)
		N(15)—C(8)—C(7)	124.5(2)

planar furazan rings (*F*) (six in molecule **2** and eight in molecule **3**) linked with azo-bridges (—*F*—N=N—*F*—). The azo fragment in both molecules has a *trans*-configuration like in 16-membered macrocycle **1** (see Ref. 2). However, the orientation of the N=N bond with respect to the endocyclic C=N bond (the nearest C=N bond of the furazan ring) changes noticeably as the number of fragments in the macrocycles increases. For example, in the each diazenofurazan fragment of molecule **1**, the orientation of the bonds mentioned is *sc-ap* (the N=N—C=N torsion angles are ~50—56° and 175—177°); three different types of orientation are found in molecule **2** (in its symmetrically independent part): *sc-ap*, *sc-sp*, and *sp-ap*; four different types, *sc-ap*, *sc-sp*, *sp-ap*, and *ap-ap*, are found in molecule **4**, and, as can be seen from Table 3, structures **2** and **3** contain two practically planar azofurazan fragments, the *F*2(*F*2a)—N=N—*F*3(*F*3a) fragment in **2** and the *F*1(*F*1a)—N=N—*F*2(*F*2a) fragment in **3**. Unlike molecule **1**, which has a saddle-shaped form,[2] molecule **2** is a truncated cone in which the *F*1 and *F*1a furazan cycles form the truncated part (the O(3)...O(3a) distance is equal to 3.071(4) Å) and the base of the cone is composed of the two *F*2—*F*3 and *F*2a—*F*3a furazan fragments. Molecule **3** has a chair conformation in which

Table 3. Torsion (φ) and dihedral (τ) angles in the azofurazan fragments (the symmetrically independent part of the molecule) of macrocycles **2** and **3**

Molecule **2**				Molecule **3**			
Cycle	τ/deg	Fragment	φ/deg	Cycle	τ/deg	Fragment	φ/deg
*F*1—*F*2	54.5	N(6)—C(5)—N(6)—N(7)	39.1	*F*1a—*F*4	112.6	N(1a)—C(1a)—N(16)—N(15)	−43.7
		N(9)—C(8)—N(7)—N(6)	16.9			N(14)—C(8)—N(15)—N(16)	−26.4
*F*2—*F*3	8.6	N(11)—C(12)—N(13)—N(14)	−1.5	*F*1—*F*2	7.2	N(2)—C(2)—N(3)—N(4)	173.2
		N(16)—C(15)—N(14)—N(13)	−175.6			N(5)—C(3)—N(4)—N(3)	11.4
*F*3—*F*1a	82.9	N(18)—C(19)—N(20)—N(21)	65.2	*F*2—*F*3	117.7	N(6)—C(4)—N(7)—N(8)	−156.3
		N(2a)—C(1a)—N(21)—N(20)	−159.4			N(9)—C(5)—N(8)—N(7)	37.5
*F*1—*F*1a	29.9			*F*3—*F*4	13.3	N(10)—C(6)—N(11)—N(12)	−168.9
						N(13)—C(7)—N(12)—N(11)	155.2

the seat is formed by the two *F*3—*F*4 and *F*3a—*F*4a coplanar azofurazan fragments, and the *F*1—*F*2 and *F*1a—*F*2a fragments compose the edges. In this connection it is interesting to note that in the crystals of macrocycles **1**—**3**, the calculated density decreases as the number of fragments increases (1.80, 1.74, and 1.70 g cm^{-3}, respectively). The geometrical parameters of the furazan cycles in both molecules are close to the tabular values calculated for substituted furazans[6] (C—C, 1.428 Å; C—N, 1.298 Å; N—O, 1.385 Å) and the C—N and N=N bond lengths in the azo fragments are in good agreement with the values of 1.428(2) and 1.247(2) Å determined for the similar bonds in the previously studied azobenzene.[7] The exocyclic bond angles at the C atoms (127—134°) in molecules **2** and **3** are significantly increased. The packing of the molecules in the crystal is of the parquet type. The intermolecular contacts are close to the sums of van der Waals radii of the corresponding atoms.

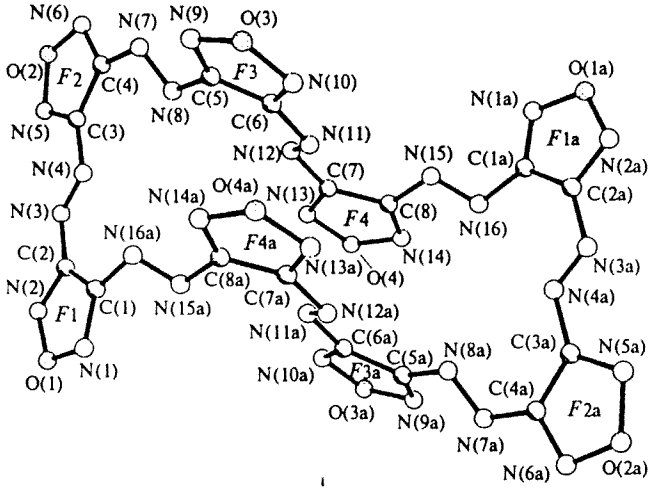


Fig. 2. Structure of molecule **3**.

Experimental

TLC control was carried out on Silufol UV-254 plates with CH_2Cl_2—hexane (3 : 1) as the eluent. The IR spectrum of compound **6** was recorded on a UR-20 instrument in KBr pellets.

Macrocyclic compounds **1**—**4** synthesized had physicochemical characteristics identical to those of previously studied samples.[1]

Synthesis of macrocycles 1—4 (general procedure). A mixture of diamine and DBI in MeCN was stirred at ~20 °C for 24 h. The precipitate that formed was filtered off and washed with a small amount of CH_2Cl_2. The mother liquor was evaporated and 5—10 mL of C_6H_6 was added to the residue. Column chromatography on LS 40/100μ silica gel (or its mixture with LS 100/250μ silica gel, 1 : 1), with C_6H_6 as the eluent afforded the individual macrocycles or their mixtures: **1** (R_f 0.68), **2** (R_f 0.51), **3** (R_f 0.42), **4** (R_f 0.79), and **5** (R_f 0.63).

Tetradiazenofurazan macrocycle 1. ***A.*** Compound **1** was obtained from DAAF (3 g, 15 mmol), DBI (11 g, 37 mmol), and MeCN (900 mL) in 88 % yield (2.60 g).

B. Compound **1** was obtained from DAAF (0.1 g, 1 mmol), DBI (1.74 g, 6 mmol), and MeCN (30 mL) in 72 % yield (0.07 g).

Tetra- (1), hexa-(2), and octadiazenofurazan (3) macrocycles were obtained from DAAF (1 g, 5 mmol), DBI (10 g, 33 mmol), and MeCN (20 mL). Compound **1** was isolated by the general procedure. For the isolation of products **2** and **3**, the residue that was not dissolved in C_6H_6 (see the general procedure), was washed with hot C_6H_6 (50 mL) and the solution was evaporated to afford compound **2**. The solid residue after the extraction of **2** was refluxed in H_2O (200 mL) for 30 min, and the insoluble residue was filtered off and washed with a small amount of C_6H_6. Column chromatography on LS 40/100 silica gel with C_6H_6 as the eluent afforded compound **3**. The yields of **1**, **2**, and **3** were 0.49 g (50 %), 0.34 g (35 %), and 0.08 g (8 %), respectively.

Tridiazenofurazan macrocycle 4. DBI was added in two portions, first, 3.5 g (12.2 mmol) then 1 g (3.5 mmol) after 1 h, to a solution of DAF (0.5 g, 5 mmol) in MeOH (50 mL). The mixture was kept for 4 h, the precipitate that formed was filtered off, the mother liquor was evaporated, the residue was extracted with C_6H_6 (20 mL), and the solution was concentrated to 1/2 of its initial volume. Column chromatography on silica gel (see the general procedure) afforded 0.06 g (12.5 %) of **4**.

4,4'-Bis(4-aminofurazanyl-3-azo)-3,3'-azofurazan (6) was prepared from DAAF (0.2 g, 1 mmol), DBI (0.88 g, 2.5 mmol), and C_6H_6 (60 mL). The reaction mixture was kept for ~72 h, the precipitate that formed was filtered off, the mother liquor was

Table 4. Atomic coordinates (×10) and their equivalent temperature factors (U_{eq}×10) in molecules **2** and **3**

Atom	x	y	z	U_{eq}/Å^2
		Molecule **2**		
C(1)	11261(2)	8376(5)	8674(2)	19(1)
N(2)	11254(2)	10335(4)	8474(2)	22(1)
O(3)	10581(1)	11038(4)	8351(2)	26(1)
N(4)	10156(2)	9494(4)	8471(2)	23(1)
C(5)	10576(2)	7861(5)	8669(2)	18(1)
N(6)	10376(2)	5981(4)	8926(2)	18(1)
N(7)	9724(2)	5569(4)	8536(2)	18(1)
C(8)	9492(2)	3808(5)	8835(2)	17(1)
N(9)	9819(2)	2950(4)	9535(2)	22(1)
O(10)	9365(1)	1356(3)	9543(2)	23(1)
N(11)	8761(2)	1245(4)	8849(2)	21(1)
C(12)	8837(2)	2765(5)	8414(2)	16(1)
N(13)	8371(2)	3296(4)	7633(2)	18(1)
N(14)	7837(2)	2119(4)	7338(2)	22(1)
C(15)	7441(2)	2675(5)	6535(2)	20(1)
N(16)	6837(2)	1749(4)	6123(2)	24(1)
O(17)	6611(1)	2590(4)	5376(2)	27(1)
N(18)	7090(2)	4084(5)	5335(2)	25(1)
C(19)	7592(2)	4140(5)	6037(2)	20(1)
N(20)	8232(2)	5334(4)	6228(2)	18(1)
N(21)	8102(2)	7251(4)	6160(2)	22(1)

Atom	x	y	z	U_{eq}/Å^2
		Molecule **3**		
O(1)	−3072(2)	5511(2)	9424(1)	67(1)
O(2)	−5854(2)	1066(2)	5411(2)	71(1)
O(3)	−3040(2)	5596(2)	1966(1)	71(1)
O(4)	1592(1)	2422(1)	6096(1)	58(1)
N(1)	−2660(2)	6084(2)	8516(2)	61(1)
N(2)	−3628(2)	4491(2)	9101(2)	60(1)
N(3)	−4140(2)	3440(2)	7459(2)	57(1)
N(4)	−4171(2)	3518(2)	6423(2)	51(1)
N(5)	−5586(2)	1743(2)	6302(2)	60(1)
N(6)	−5536(2)	1472(2)	4390(2)	68(1)
N(7)	−4397(2)	3014(2)	3768(2)	60(1)
N(8)	−3468(2)	3553(2)	4101(2)	51(1)
N(9)	−3777(2)	4888(2)	2545(2)	62(1)
N(10)	−1858(2)	5438(2)	2338(2)	62(1)
N(11)	−753(2)	4325(2)	3703(1)	47(1)
N(12)	−822(2)	3431(2)	4311(2)	48(1)
N(13)	383(2)	2549(2)	5800(2)	56(1)
N(14)	2258(2)	2949(2)	5311(1)	51(1)
N(15)	1740(2)	3874(2)	3500(1)	48(1)
N(16)	2753(2)	4258(2)	3485(2)	56(1)
C(1)	−2975(2)	5428(2)	7645(2)	45(1)
C(2)	−3594(2)	4434(2)	8006(2)	47(1)
C(3)	−4761(2)	2541(2)	5846(2)	46(1)
C(4)	−4849(2)	2376(2)	4656(2)	51(1)
C(5)	−3059(2)	4296(2)	3257(2)	46(1)
C(6)	−1861(2)	4644(2)	3133(2)	45(1)
C(7)	309(2)	3143(2)	4856(2)	43(1)
C(8)	1483(2)	3393(2)	4556(2)	39(1)

concentrated *in vacuo* and chromatographed on LS 100/250 silica gel column using C_6H_6—EtOAc (5 : 1) as the eluent. Compound **1** (0.04 g, 20 %) was isolated from the fraction with R_f 0.85. The fraction containing a mixture of DAAF (R_f 0.31) and **6** (R_f 0.17) was chromatographed on LS 5/40μ silica gel plates using C_6H_6—EtOAc (5 : 1) as the eluent to afford 0.03 g (15 %) of **6**. IR, ν/cm^{-1}: 3455, 3335, 1630, 1510, 1430, 1240, 1035, 770.

X-ray structural study of compounds 2 and 3. Monocrystals **2** and **3** obtained by crystallization from C_6H_6 and HNO_3 (d = 1.5 g cm^{-3}), respectively, are monoclinic; for **2** at 153 K a = 20.231(17) Å, b = 6.486(7) Å, c = 18.220(19) Å, β = 113.08(2)°, V = 2199(4) Å^3, Z = 4, d = 1.740 g cm^{-3}, $C2/c$ space group, $C_{12}N_{24}O_6$, M = 576.36; for **3** at 296 K, a = 11.230(9) Å, b = 11.355(3) Å, c = 11.828(8) Å, β = 95.44(6)°, V = 1501.5 Å^3, Z = 2, d = 1.700 g cm^{-3}, $P21/n$ space group $C_{16}N_{32}O_8$, M = 768.48. Cell parameters and intensities of 1565 (for **2**) and 2137 (for **3**) independent reflections with $I > 2\sigma(I)$ were measured on Siemens P3/PC (**2**) and Enraf Nonius KAD-4 (**3**) automatic diffractometers (λ(Mo-Kα), graphite monochromator, θ/2θ-scanning , 2θ = 60°). The structures were solved by the direct method and refined by the least squares method with a full-matrix anisotropic approximation. The final divergence factors were R = 0.065, R_w = 0.065 (**2**); R = 0.0405, R_w = 0.0422 (**3**). All calculations were carried out using a SHELXTL PLUS program (PC Version).[8] The atomic coordinates and their temperature factors are given in Table 4.

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