Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,2,13,14,14a,15,16,17,18,18a-Decahydro-1,14-methano-4*H*,6*H*,8*H*-1,3,5-oxadiazino[3′,4′:3,3a]benzimidazo[1,7a-*b*][2,4]benzodiazepine-6,19-dione

Nengfang She[a]* and Hailing Xi[b]

[a]Key Laboratory of Pesticides and Chemical Biology of the Ministry of Education, College of Chemistry, Central China Normal University, Wuhan 430079, People's Republic of China, and [b]6th Department, Research Institute of Chemical Defence, Beijing 102205, People's Republic of China
Correspondence e-mail: wuhannshe@yahoo.com.cn

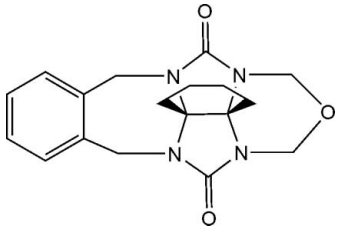
Received 20 October 2007; accepted 20 October 2007

Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.002 Å; R factor = 0.045; wR factor = 0.129; data-to-parameter ratio = 15.5.

In the title compound, $C_{18}H_{20}N_4O_3$, a glycoluril derivative, the oxadiazinane six-membered ring displays a chair conformation and the bridgehead cyclohexane ring a boat conformation. In the crystal structure, intermolecular C—H···O hydrogen bonds may help to establish the packing.

Related literature

For related structures, see: Fettinger *et al.* (2004); Cao *et al.* (2006). For background, see: Jansen *et al.* (2001); Wu *et al.* (2002); Reek *et al.* (2003).



Experimental

Crystal data

$C_{18}H_{20}N_4O_3$
M_r = 340.38
Monoclinic, $P2_1/n$
a = 11.8315 (12) Å
b = 11.3603 (11) Å
c = 11.9716 (12) Å
β = 90.261 (2)°
V = 1609.1 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 297 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART 4K CCD diffractometer
Absorption correction: none
9429 measured reflections
3494 independent reflections
2964 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.129
S = 1.05
3494 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15B···O1^{i}	0.97	2.49	3.3991 (18)	156
C17—H17A···O2^{ii}	0.97	2.54	3.510 (2)	174
C12—H12B···O1^{i}	0.97	2.60	3.4963 (18)	155
C3—H3···O1^{iii}	0.93	2.45	3.3144 (19)	155

Symmetry codes: (i) $-x+2, -y, -z+1$; (ii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x+2, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Bruker, 2001).

The authors thank Dr Xiang-Gao Meng for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2603).

References

Bruker (2001). *SMART* (Version 5.628), *SAINT* (Version 6.45) and *SHELXTL* (Version 6.12). Bruker AXS Inc., Madison, Wisconsin, USA.
Cao, L.-P., Gao, M. & Zhou, B.-H. (2006). *Acta Cryst.* E**62**, o5419–o5420.
Fettinger, J. C., Wu, A. & Isaacs, L. (2004). *Acta Cryst.* E**60**, o1814–o1816.
Jansen, R. J., Gelder, R., Rowan, A. E., Scheeren, H. W. & Nolte, R. J. M. (2001). *J. Org. Chem.* **66**, 2643–2653.
Reek, J. N. H., Elemans, J. A. A. W., Gelder, R., Beurskens, P. T. & Nolte, R. J. M. (2003). *Tetrahedron*, **59**, 2003, 175–185.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Wu, A., Chakraborty, A., Witt, D., Lagona, J., Damkaci, F., Ofori, M. A., Chiles, J. K., Fettinger, J. C. & Isaacs, L. (2002). *J. Org. Chem.* **67**, 5817–5830.

  doi:10.1107/S1600536807052038

supplementary materials

Acta Cryst. (2007). E**63**, o4440 [**doi:10.1107/S1600536807052038**]

1,2,13,14,14a,15,16,17,18,18a-Decahydro-1,14-methano-4*H*,6*H*,8*H*-1,3,5-oxadiazino[3',4':3,3a]benzimidazo[1,7a-*b*][2,4]benzodiazepine-6,19-dione

N. She and H. Xi

Comment

Glycolurils, due to their special pre-formed skeletal structures, are widely used as platforms or building blocks to construct a series of compounds with more sophisticated structures (e. g. Reek *et al.*, 2003). In recent years a series of receptors derived from glycoluril have been developed (Jansen *et al.*, 2001).

We report here the structure of the title glycoluril derivative, (I) (Fig. 1), which is an important intermediate for the preparation of glycoluril receptors (Wu *et al.*, 2002). The bond lengths and angles present in (I) show no unusual features and are similar to those found in other similar compounds (Fettinger *et al.*, 2004; Cao *et al.*, 2006).

The imidazole ring A (N1/N3/C9/C11/C16) and ring B (N2/N4/C10–11/C16) are close to flat, the maximum deviation from the mean plane being 0.085 (2) Å and 0.093 (2) Å for atom C9 or N2. The dihedral angle between them is 72.28 (7)°. The C_3N_2O oxadiazinane six-membered ring displays a chair conformation.

In the crystal, weak intermolecular C—H···O hydrogen bonds lead to the formation of a tape-like structure (Fig. 2).

Experimental

The title compound was synthesized according to the procedure of Wu *et al.* (2002). Colourless blocks of (I) were obtained by slow evaporation of a dichloromethane solution at 283 K.

Refinement

The H atoms were positioned geometrically, with C—H = 0.93 and 0.97 Å for aromatic and methylene H, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

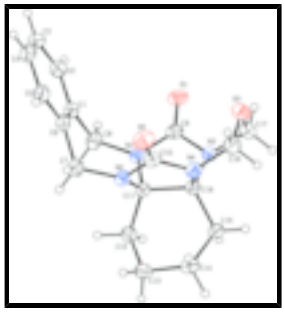


Fig. 1. The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level for the non-hydrogen atoms.

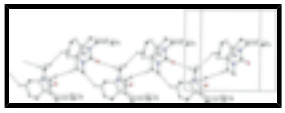


Fig. 2. A packing diagram for (I). C—H···O hydrogen bonds are shown as dashed lines.

1,2,13,14,14*a*,15,16,17,18,18*a*-Decahydro-1,14-methano-4H,6*H*,8*H*- 1,3,5-oxadiazino[3',4':3,3a]benzimidazo[1,7a-b][2,4]benzodiazepine- 6,19-dione

Crystal data

$C_{18}H_{20}N_4O_3$	F_{000} = 720
M_r = 340.38	D_x = 1.405 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 4769 reflections
a = 11.8315 (12) Å	θ = 2.4–28.2º
b = 11.3603 (11) Å	μ = 0.10 mm^{-1}
c = 11.9716 (12) Å	T = 297 (2) K
β = 90.261 (2)º	Block, colorless
V = 1609.1 (3) Å^3	0.30 × 0.20 × 0.20 mm
Z = 4	

Data collection

Bruker SMART 4K CCD diffractometer	2964 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.020
Monochromator: graphite	θ_{max} = 27.0º
T = 297(2) K	θ_{min} = 2.4º
ω scans	h = −13→15
Absorption correction: none	k = −10→14
9429 measured reflections	l = −14→15
3494 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.045	H-atom parameters constrained
$wR(F^2)$ = 0.129	$w = 1/[\sigma^2(F_o^2) + (0.0769P)^2 + 0.2493P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max}$ = 0.001
3494 reflections	$\Delta\rho_{max}$ = 0.22 e Å^{-3}
226 parameters	$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N2	1.00013 (9)	0.16297 (9)	0.17388 (9)	0.0371 (3)
N3	0.87562 (9)	0.04324 (10)	0.39525 (9)	0.0393 (3)
O1	0.93433 (10)	0.18108 (9)	0.52572 (8)	0.0525 (3)
C11	1.02131 (10)	0.07801 (11)	0.26298 (10)	0.0329 (3)
C9	0.94842 (11)	0.12802 (11)	0.43866 (11)	0.0384 (3)
O2	0.84406 (10)	0.26030 (10)	0.10290 (9)	0.0566 (3)
N1	1.03911 (9)	0.13619 (10)	0.36993 (9)	0.0380 (3)
O3	0.70042 (9)	0.13063 (10)	0.34834 (11)	0.0599 (3)
N4	0.82993 (9)	0.08765 (10)	0.20448 (10)	0.0409 (3)
C16	0.90377 (10)	0.01906 (11)	0.27860 (10)	0.0341 (3)
C10	0.88658 (12)	0.18055 (12)	0.15638 (11)	0.0399 (3)
C12	1.11293 (11)	−0.01106 (13)	0.23557 (12)	0.0435 (3)
H12A	1.1827	0.0304	0.2195	0.052*
H12B	1.1261	−0.0607	0.3002	0.052*
C15	0.90251 (12)	−0.11112 (11)	0.24948 (12)	0.0395 (3)
H15A	0.8251	−0.1391	0.2461	0.047*
H15B	0.9420	−0.1553	0.3069	0.047*
C6	1.08589 (11)	0.35691 (12)	0.22752 (12)	0.0419 (3)
C13	1.08184 (14)	−0.08793 (14)	0.13630 (14)	0.0526 (4)
H13A	1.1315	−0.1559	0.1353	0.063*
H13B	1.0947	−0.0438	0.0682	0.063*
C7	1.08185 (13)	0.25468 (13)	0.14646 (11)	0.0447 (3)
H7A	1.0642	0.2850	0.0727	0.054*
H7B	1.1564	0.2194	0.1431	0.054*
C8	1.13119 (12)	0.21882 (13)	0.38893 (12)	0.0460 (3)
H8A	1.1995	0.1872	0.3559	0.055*
H8B	1.1442	0.2258	0.4687	0.055*
C17	0.75673 (13)	0.04987 (15)	0.42045 (14)	0.0538 (4)
H17A	0.7231	−0.0275	0.4123	0.065*
H17B	0.7471	0.0747	0.4974	0.065*
C5	1.06832 (13)	0.47048 (14)	0.18786 (16)	0.0544 (4)
H5	1.0519	0.4822	0.1126	0.065*
C1	1.10963 (11)	0.34032 (13)	0.34123 (12)	0.0429 (3)

C18	0.71283 (12)	0.09427 (15)	0.23565 (15)	0.0544 (4)
H18A	0.6741	0.1496	0.1870	0.065*
H18B	0.6780	0.0177	0.2258	0.065*
C14	0.95944 (13)	−0.13044 (13)	0.13732 (12)	0.0468 (3)
H14A	0.9172	−0.0890	0.0799	0.056*
H14B	0.9576	−0.2137	0.1194	0.056*
C3	1.09754 (15)	0.55057 (15)	0.37046 (19)	0.0662 (5)
H3	1.1015	0.6148	0.4184	0.079*
C4	1.07500 (14)	0.56673 (15)	0.2592 (2)	0.0672 (5)
H4	1.0641	0.6423	0.2313	0.081*
C2	1.11438 (14)	0.43785 (15)	0.41086 (16)	0.0569 (4)
H2	1.1292	0.4272	0.4865	0.068*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N2	0.0430 (6)	0.0330 (5)	0.0352 (5)	−0.0025 (5)	−0.0016 (4)	0.0022 (4)
N3	0.0402 (6)	0.0360 (6)	0.0417 (6)	−0.0005 (5)	0.0086 (4)	−0.0033 (5)
O1	0.0746 (7)	0.0445 (6)	0.0384 (5)	0.0023 (5)	0.0057 (5)	−0.0076 (4)
C11	0.0354 (6)	0.0303 (6)	0.0331 (6)	−0.0004 (5)	−0.0008 (5)	0.0000 (5)
C9	0.0487 (8)	0.0312 (6)	0.0354 (6)	0.0035 (5)	0.0003 (5)	0.0010 (5)
O2	0.0676 (7)	0.0432 (6)	0.0590 (7)	0.0108 (5)	−0.0153 (5)	0.0088 (5)
N1	0.0428 (6)	0.0380 (6)	0.0332 (5)	−0.0068 (5)	−0.0018 (4)	−0.0007 (4)
O3	0.0417 (6)	0.0529 (7)	0.0850 (8)	0.0110 (5)	0.0086 (5)	−0.0094 (6)
N4	0.0357 (6)	0.0355 (6)	0.0514 (7)	0.0032 (4)	−0.0069 (5)	0.0001 (5)
C16	0.0334 (6)	0.0308 (6)	0.0380 (6)	0.0016 (5)	0.0003 (5)	−0.0007 (5)
C10	0.0479 (7)	0.0324 (7)	0.0393 (7)	0.0046 (5)	−0.0071 (5)	−0.0042 (5)
C12	0.0364 (7)	0.0408 (7)	0.0533 (8)	0.0045 (6)	0.0057 (6)	0.0031 (6)
C15	0.0419 (7)	0.0294 (6)	0.0471 (7)	−0.0013 (5)	0.0005 (5)	−0.0016 (5)
C6	0.0343 (6)	0.0362 (7)	0.0553 (8)	−0.0047 (5)	0.0063 (6)	0.0020 (6)
C13	0.0620 (9)	0.0405 (8)	0.0553 (9)	0.0048 (7)	0.0191 (7)	−0.0053 (7)
C7	0.0531 (8)	0.0430 (8)	0.0381 (7)	−0.0070 (6)	0.0059 (6)	0.0051 (6)
C8	0.0472 (8)	0.0471 (8)	0.0437 (7)	−0.0101 (6)	−0.0076 (6)	−0.0024 (6)
C17	0.0461 (8)	0.0502 (9)	0.0652 (10)	−0.0006 (7)	0.0181 (7)	−0.0042 (7)
C5	0.0410 (8)	0.0422 (8)	0.0801 (11)	−0.0021 (6)	0.0037 (7)	0.0106 (8)
C1	0.0367 (7)	0.0406 (7)	0.0514 (8)	−0.0081 (6)	0.0076 (6)	−0.0064 (6)
C18	0.0357 (7)	0.0482 (9)	0.0791 (11)	0.0037 (6)	−0.0071 (7)	−0.0054 (8)
C14	0.0612 (9)	0.0366 (7)	0.0427 (7)	0.0046 (6)	−0.0013 (6)	−0.0060 (6)
C3	0.0530 (9)	0.0454 (9)	0.1005 (15)	−0.0072 (7)	0.0239 (9)	−0.0274 (9)
C4	0.0434 (9)	0.0354 (8)	0.1228 (18)	0.0020 (6)	0.0160 (9)	0.0013 (9)
C2	0.0521 (9)	0.0534 (9)	0.0653 (10)	−0.0136 (7)	0.0150 (7)	−0.0190 (8)

Geometric parameters (Å, °)

N2—C10	1.3734 (17)	C6—C5	1.390 (2)
N2—C11	1.4593 (16)	C6—C1	1.401 (2)
N2—C7	1.4598 (17)	C6—C7	1.514 (2)
N3—C9	1.3912 (17)	C13—C14	1.527 (2)
N3—C17	1.4419 (18)	C13—H13A	0.9700

N3—C16	1.4631 (17)	C13—H13B	0.9700
O1—C9	1.2161 (16)	C7—H7A	0.9700
C11—N1	1.4554 (16)	C7—H7B	0.9700
C11—C12	1.5198 (18)	C8—C1	1.515 (2)
C11—C16	1.5556 (17)	C8—H8A	0.9700
C9—N1	1.3582 (17)	C8—H8B	0.9700
O2—C10	1.2169 (16)	C17—H17A	0.9700
N1—C8	1.4552 (17)	C17—H17B	0.9700
O3—C18	1.419 (2)	C5—C4	1.390 (3)
O3—C17	1.423 (2)	C5—H5	0.9300
N4—C10	1.3777 (19)	C1—C2	1.387 (2)
N4—C18	1.4384 (18)	C18—H18A	0.9700
N4—C16	1.4665 (16)	C18—H18B	0.9700
C16—C15	1.5195 (18)	C14—H14A	0.9700
C12—C13	1.519 (2)	C14—H14B	0.9700
C12—H12A	0.9700	C3—C4	1.369 (3)
C12—H12B	0.9700	C3—C2	1.383 (3)
C15—C14	1.521 (2)	C3—H3	0.9300
C15—H15A	0.9700	C4—H4	0.9300
C15—H15B	0.9700	C2—H2	0.9300
C10—N2—C11	111.86 (10)	C12—C13—H13B	108.8
C10—N2—C7	120.69 (11)	C14—C13—H13B	108.8
C11—N2—C7	121.65 (11)	H13A—C13—H13B	107.7
C9—N3—C17	119.25 (11)	N2—C7—C6	114.99 (11)
C9—N3—C16	110.08 (10)	N2—C7—H7A	108.5
C17—N3—C16	115.85 (11)	C6—C7—H7A	108.5
N1—C11—N2	111.49 (10)	N2—C7—H7B	108.5
N1—C11—C12	113.07 (10)	C6—C7—H7B	108.5
N2—C11—C12	113.75 (10)	H7A—C7—H7B	107.5
N1—C11—C16	102.45 (9)	N1—C8—C1	113.84 (11)
N2—C11—C16	102.83 (9)	N1—C8—H8A	108.8
C12—C11—C16	112.23 (10)	C1—C8—H8A	108.8
O1—C9—N1	126.66 (13)	N1—C8—H8B	108.8
O1—C9—N3	125.18 (13)	C1—C8—H8B	108.8
N1—C9—N3	108.09 (11)	H8A—C8—H8B	107.7
C9—N1—C8	122.84 (11)	O3—C17—N3	111.18 (12)
C9—N1—C11	112.98 (10)	O3—C17—H17A	109.4
C8—N1—C11	122.39 (11)	N3—C17—H17A	109.4
C18—O3—C17	109.80 (11)	O3—C17—H17B	109.4
C10—N4—C18	122.64 (12)	N3—C17—H17B	109.4
C10—N4—C16	111.74 (10)	H17A—C17—H17B	108.0
C18—N4—C16	116.27 (12)	C4—C5—C6	120.82 (18)
N3—C16—N4	109.89 (10)	C4—C5—H5	119.6
N3—C16—C15	113.56 (11)	C6—C5—H5	119.6
N4—C16—C15	111.91 (11)	C2—C1—C6	118.92 (15)
N3—C16—C11	103.97 (10)	C2—C1—C8	119.66 (14)
N4—C16—C11	103.23 (10)	C6—C1—C8	121.43 (12)
C15—C16—C11	113.53 (10)	O3—C18—N4	111.45 (12)
O2—C10—N2	126.18 (14)	O3—C18—H18A	109.3

O2—C10—N4	126.12 (13)	N4—C18—H18A	109.3
N2—C10—N4	107.59 (11)	O3—C18—H18B	109.3
C13—C12—C11	112.42 (12)	N4—C18—H18B	109.3
C13—C12—H12A	109.1	H18A—C18—H18B	108.0
C11—C12—H12A	109.1	C15—C14—C13	112.66 (12)
C13—C12—H12B	109.1	C15—C14—H14A	109.1
C11—C12—H12B	109.1	C13—C14—H14A	109.1
H12A—C12—H12B	107.9	C15—C14—H14B	109.1
C16—C15—C14	109.82 (11)	C13—C14—H14B	109.1
C16—C15—H15A	109.7	H14A—C14—H14B	107.8
C14—C15—H15A	109.7	C4—C3—C2	119.43 (16)
C16—C15—H15B	109.7	C4—C3—H3	120.3
C14—C15—H15B	109.7	C2—C3—H3	120.3
H15A—C15—H15B	108.2	C3—C4—C5	120.17 (17)
C5—C6—C1	119.05 (14)	C3—C4—H4	119.9
C5—C6—C7	119.26 (14)	C5—C4—H4	119.9
C1—C6—C7	121.67 (13)	C3—C2—C1	121.59 (18)
C12—C13—C14	113.71 (12)	C3—C2—H2	119.2
C12—C13—H13A	108.8	C1—C2—H2	119.2
C14—C13—H13A	108.8		
C10—N2—C11—N1	−94.60 (12)	C7—N2—C10—O2	12.3 (2)
C7—N2—C11—N1	58.67 (15)	C11—N2—C10—N4	−17.78 (14)
C10—N2—C11—C12	136.10 (12)	C7—N2—C10—N4	−171.35 (11)
C7—N2—C11—C12	−70.62 (15)	C18—N4—C10—O2	−24.9 (2)
C10—N2—C11—C16	14.50 (13)	C16—N4—C10—O2	−170.16 (13)
C7—N2—C11—C16	167.77 (11)	C18—N4—C10—N2	158.67 (12)
C17—N3—C9—O1	28.9 (2)	C16—N4—C10—N2	13.46 (15)
C16—N3—C9—O1	166.34 (13)	N1—C11—C12—C13	168.61 (11)
C17—N3—C9—N1	−154.01 (12)	N2—C11—C12—C13	−62.90 (15)
C16—N3—C9—N1	−16.56 (14)	C16—C11—C12—C13	53.32 (15)
O1—C9—N1—C8	−4.4 (2)	N3—C16—C15—C14	−166.31 (11)
N3—C9—N1—C8	178.55 (11)	N4—C16—C15—C14	68.56 (14)
O1—C9—N1—C11	−169.48 (13)	C11—C16—C15—C14	−47.82 (15)
N3—C9—N1—C11	13.47 (15)	C11—C12—C13—C14	−42.71 (18)
N2—C11—N1—C9	104.29 (12)	C10—N2—C7—C6	75.03 (16)
C12—C11—N1—C9	−126.05 (12)	C11—N2—C7—C6	−75.93 (16)
C16—C11—N1—C9	−5.05 (13)	C5—C6—C7—N2	−123.34 (14)
N2—C11—N1—C8	−60.86 (15)	C1—C6—C7—N2	58.23 (18)
C12—C11—N1—C8	68.80 (16)	C9—N1—C8—C1	−85.48 (16)
C16—C11—N1—C8	−170.20 (12)	C11—N1—C8—C1	78.21 (16)
C9—N3—C16—N4	−96.99 (12)	C18—O3—C17—N3	59.77 (16)
C17—N3—C16—N4	42.05 (15)	C9—N3—C17—O3	82.31 (16)
C9—N3—C16—C15	136.81 (11)	C16—N3—C17—O3	−52.80 (16)
C17—N3—C16—C15	−84.16 (14)	C1—C6—C5—C4	0.5 (2)
C9—N3—C16—C11	12.94 (13)	C7—C6—C5—C4	−177.93 (14)
C17—N3—C16—C11	151.98 (11)	C5—C6—C1—C2	0.3 (2)
C10—N4—C16—N3	106.11 (12)	C7—C6—C1—C2	178.71 (13)
C18—N4—C16—N3	−41.49 (15)	C5—C6—C1—C8	−179.11 (13)
C10—N4—C16—C15	−126.76 (12)	C7—C6—C1—C8	−0.7 (2)

C18—N4—C16—C15	85.64 (14)	N1—C8—C1—C2	123.37 (14)
C10—N4—C16—C11	−4.30 (14)	N1—C8—C1—C6	−57.23 (18)
C18—N4—C16—C11	−151.90 (11)	C17—O3—C18—N4	−59.14 (16)
N1—C11—C16—N3	−4.75 (12)	C10—N4—C18—O3	−92.18 (16)
N2—C11—C16—N3	−120.54 (10)	C16—N4—C18—O3	51.59 (17)
C12—C11—C16—N3	116.83 (11)	C16—C15—C14—C13	59.16 (16)
N1—C11—C16—N4	110.00 (10)	C12—C13—C14—C15	−13.33 (18)
N2—C11—C16—N4	−5.79 (12)	C2—C3—C4—C5	0.5 (3)
C12—C11—C16—N4	−128.42 (11)	C6—C5—C4—C3	−0.9 (2)
N1—C11—C16—C15	−128.64 (11)	C4—C3—C2—C1	0.4 (3)
N2—C11—C16—C15	115.58 (11)	C6—C1—C2—C3	−0.7 (2)
C12—C11—C16—C15	−7.06 (15)	C8—C1—C2—C3	178.67 (14)
C11—N2—C10—O2	165.84 (13)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15B···O1^{i}	0.97	2.49	3.3991 (18)	156
C17—H17A···O2^{ii}	0.97	2.54	3.510 (2)	174
C12—H12B···O1^{i}	0.97	2.60	3.4963 (18)	155
C3—H3···O1^{iii}	0.93	2.45	3.3144 (19)	155

Symmetry codes: (i) −*x*+2, −*y*, −*z*+1; (ii) −*x*+3/2, *y*−1/2, −*z*+1/2; (iii) −*x*+2, −*y*+1, −*z*+1.

Fig. 1

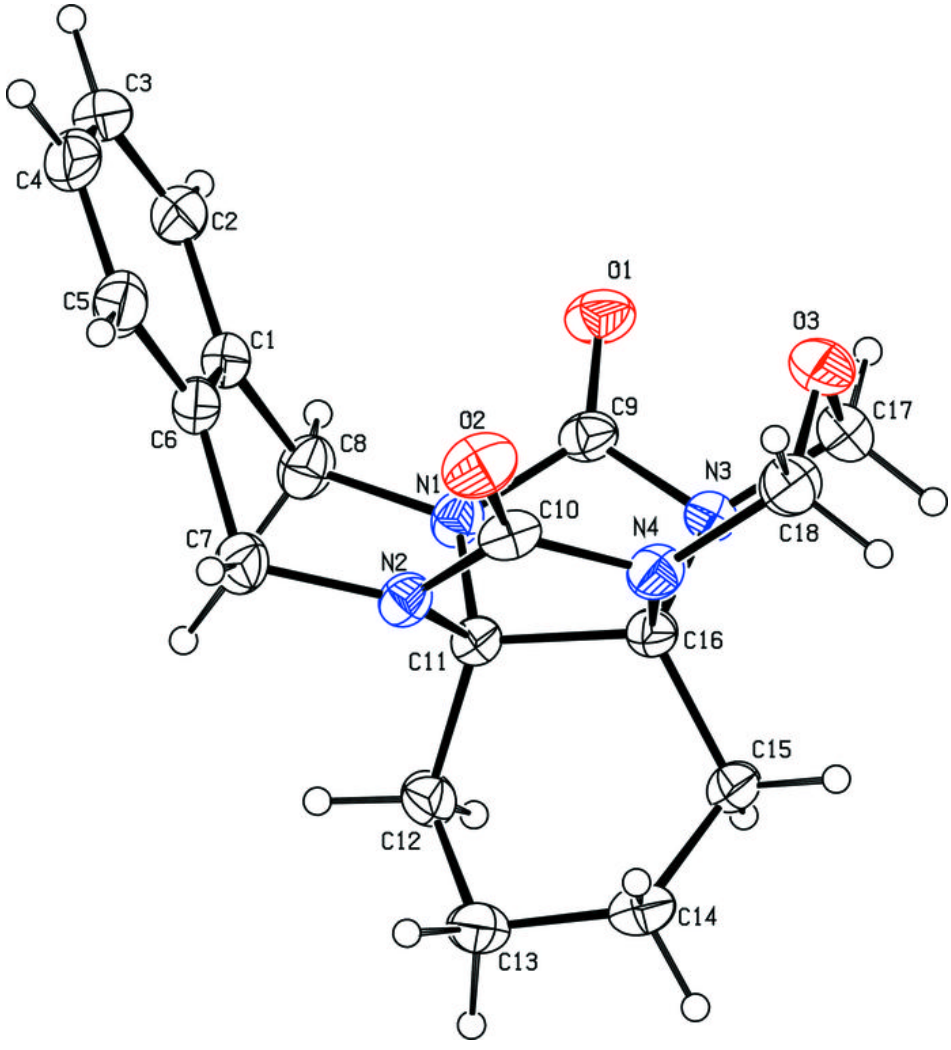

C3
C4
C2
C5
C1
O1
O3
C17
C6
C8
O2
C9
N3
N1
C10
N4
C18
C7
N2
C16
C11
C15
C12
C14
C13

Fig. 2