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Diethyl 2,6-diethyl-4,8-dioxo-2,3,6,7-tetrahydro-1*H*,5*H*-2,3a,4a,6,7a,8a-hexaazacyclopenta[*def*]fluorene-8b,8c-dicarboxylate

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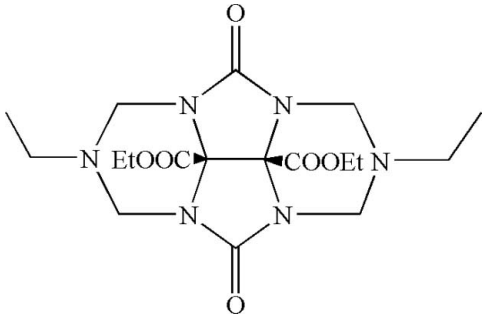
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.005 Å; R factor = 0.068; wR factor = 0.190; data-to-parameter ratio = 13.3.

The title compound, $C_{18}H_{28}N_6O_6$, is a derivative of glycoluril, with two ethyl acetate substituents on the convex face of the glycoluril system. Two equivalent six-membered rings bind the N atoms from separate rings of the glycoluril unit to form the flexible sidewalls of a molecular clip. One N atom from each ring carries an ethyl substituent. The crystal packing is stabilized by non-classical C—H···O hydrogen bonds.

Related literature

For preparation of the title compound, see: Li *et al.* (2006). For general background regarding glycoluril and its derivatives, see: Behrend *et al.* (1905); Freeman *et al.* (1981); Rebek (2005); Rowan *et al.* (1999); Wu *et al.* (2002).



Experimental

Crystal data

$C_{18}H_{28}N_6O_6$
M_r = 424.47
Monoclinic, $C2/c$
a = 20.3689 (13) Å
b = 7.8804 (5) Å
c = 25.9921 (16) Å
β = 91.697 (1)°
V = 4170.3 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 292 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART 4 K CCD area-detector diffractometer
Absorption correction: none
13315 measured reflections
3662 independent reflections
2901 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.190
S = 1.04
3662 reflections
275 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4B···O3^{i}	0.97	2.53	3.460 (4)	160

Symmetry code: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$.

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: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2270).

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supplementary materials

Acta Cryst. (2007). E**63**, o3374 [**doi:10.1107/S1600536807031819**]

Diethyl 2,6-diethyl-4,8-dioxo-2,3,6,7-tetrahydro-1*H*,5*H*-2,3a,4a,6,7a,8a-hexaazacyclopenta[*def*]fluorene-8b,8c-dicarboxylate

L.-P. Cao, Y.-Z. Wang and M. Gao

Comment

In 1905, Behrend reported that the condensation of glycoluril and formadehyde in dilute H_{Cl} yielded an insoluble polymeric material now known as Behrend's polymer (Behrend *et al.*, 1905). After 76 years, the molecular structure (obtained by heating Behrend's polymer in H_2S_O4) was disclosed by Mock and co-workers who named it cucurbituril (Freeman *et al.*, 1981). Glycoluril and its derivatives have during the past two decades established an impressive career as building block for supramolecular chemistry (Freeman *et al.*, 1981; Rebek, 2005; Rowan *et al.*, 1999; Wu *et al.*, 2002). As a part of our ongoing investigation into glycoluril derivatives (Li *et al.*, 2006), we report here the structure of the title compound (I) (Fig. 1).

The molecular structure of (I) is shown in Fig. 1. It has four fused rings - two imidazole and two triazinane rings, respectively. The crystal packing is stabilized by intermolecular non-classical C—H···O hydrogen bonds (Table 1).

Experimental

The title compound was synthesized according to the procedure of Li *et al.* (2006) in 10% isolated yield. Crystals of (I) suitable for X-ray data collection were obtained by slow evaporation of a chloroform and methaol solution in ratio of 20:1 at 293 K.

Refinement

All H atoms were positioned geometrically (C—H = 0.96–0.97 Å) and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C) (1.5U_{eq}(C) for methly) of the parent atoms.

Figures

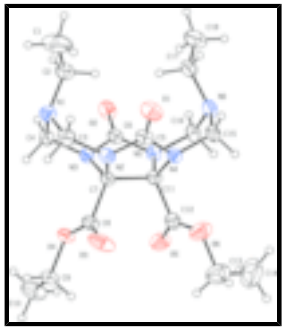


Fig. 1. View of the molecule of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented by spheres of arbitrary radius.

Diethyl 2,6-diethyl-4,8-dioxo-2,3,6,7-tetrahydro-1H,5*H*-2,3a,4a,6,7a,8a-\ hexaazacyclopenta[def]fluorene-8b,8c-dicarboxylate

Crystal data

$C_{18}H_{28}N_6O_6$	F_{000} = 1808
M_r = 424.47	D_x = 1.352 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 3350 reflections
a = 20.3689 (13) Å	θ = 2.5–22.8º
b = 7.8804 (5) Å	μ = 0.10 mm^{-1}
c = 25.9921 (16) Å	*T* = 292 (2) K
β = 91.6970 (10)º	Block, colourless
V = 4170.3 (5) Å^3	0.30 × 0.20 × 0.20 mm
Z = 8	

Data collection

Bruker SMART 4K CCD area-detector diffractometer	2901 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.031
Monochromator: graphite	θ_{max} = 25.0º
T = 292(2) K	θ_{min} = 2.0º
φ and ω scans	*h* = −24→20
Absorption correction: none	*k* = −9→9
13315 measured reflections	*l* = −30→30
3662 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
$R[F^2 > 2\sigma(F^2)]$ = 0.068	H-atom parameters constrained
$wR(F^2)$ = 0.190	$w = 1/[\sigma^2(F_o^2) + (0.0969P)^2 + 6.5727P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max} < 0.001$
3662 reflections	$\Delta\rho_{max}$ = 0.76 e Å^{-3}
275 parameters	$\Delta\rho_{min}$ = −0.50 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}
C1	0.5192 (2)	0.4727 (9)	0.3310 (2)	0.115 (2)
H1A	0.5198	0.3943	0.3027	0.172*
H1B	0.5529	0.4427	0.3559	0.172*
H1C	0.5270	0.5855	0.3186	0.172*
C2	0.45446 (17)	0.4660 (5)	0.35513 (14)	0.0613 (9)
H2A	0.4509	0.3599	0.3738	0.074*
H2B	0.4517	0.5578	0.3799	0.074*
C3	0.39338 (16)	0.6401 (4)	0.29128 (11)	0.0521 (8)
H3A	0.3668	0.6243	0.2601	0.062*
H3B	0.4368	0.6758	0.2813	0.062*
C4	0.33661 (15)	0.4321 (4)	0.33911 (11)	0.0459 (7)
H4A	0.3429	0.3321	0.3605	0.055*
H4B	0.3063	0.4023	0.3111	0.055*
C5	0.39979 (14)	0.8907 (4)	0.35146 (11)	0.0429 (7)
C6	0.31809 (13)	0.5820 (3)	0.42271 (10)	0.0374 (6)
C7	0.30321 (13)	0.7315 (3)	0.34576 (10)	0.0344 (6)
C8	0.24532 (14)	0.7504 (4)	0.30633 (11)	0.0417 (7)
C9	0.14594 (14)	0.6412 (4)	0.27281 (13)	0.0526 (8)
H9A	0.1584	0.6089	0.2384	0.063*
H9B	0.1296	0.7569	0.2716	0.063*
C10	0.09497 (19)	0.5268 (6)	0.29102 (18)	0.0849 (13)
H10A	0.1120	0.4134	0.2932	0.127*
H10B	0.0579	0.5292	0.2674	0.127*
H10C	0.0816	0.5629	0.3244	0.127*
C11	0.30001 (13)	0.8576 (3)	0.39207 (10)	0.0363 (6)
C12	0.23560 (15)	0.9608 (4)	0.39291 (12)	0.0462 (7)
C13	0.1855 (2)	1.2302 (6)	0.3808 (2)	0.0906 (14)
H13A	0.1944	1.3313	0.3610	0.109*
H13B	0.1498	1.1688	0.3637	0.109*
C14	0.1675 (3)	1.2762 (8)	0.4321 (3)	0.128 (2)
H14A	0.1501	1.1787	0.4491	0.191*
H14B	0.1348	1.3639	0.4303	0.191*
H14C	0.2055	1.3168	0.4510	0.191*

C15	0.38474 (15)	1.0349 (4)	0.43596 (12)	0.0472 (7)
H15A	0.4276	1.0836	0.4299	0.057*
H15B	0.3559	1.1264	0.4459	0.057*
C16	0.32934 (15)	0.8260 (4)	0.48422 (11)	0.0470 (7)
H16A	0.2969	0.9055	0.4963	0.056*
H16B	0.3354	0.7390	0.5103	0.056*
C17	0.44876 (16)	0.8037 (4)	0.47574 (13)	0.0542 (8)
H17A	0.4868	0.8714	0.4674	0.065*
H17B	0.4417	0.7211	0.4485	0.065*
C18	0.4623 (2)	0.7123 (5)	0.52582 (16)	0.0754 (11)
H18A	0.4609	0.7917	0.5538	0.113*
H18B	0.5050	0.6608	0.5253	0.113*
H18C	0.4296	0.6261	0.5303	0.113*
N1	0.39898 (13)	0.4795 (3)	0.31793 (9)	0.0498 (7)
N2	0.36403 (11)	0.7760 (3)	0.32213 (8)	0.0406 (6)
N3	0.30724 (11)	0.5667 (3)	0.36995 (8)	0.0359 (5)
N4	0.35879 (11)	0.9595 (3)	0.38760 (9)	0.0393 (6)
N5	0.30415 (11)	0.7466 (3)	0.43647 (8)	0.0372 (5)
N6	0.39087 (12)	0.9148 (3)	0.47816 (9)	0.0469 (6)
O1	0.45657 (11)	0.9299 (3)	0.34542 (9)	0.0636 (7)
O2	0.33390 (12)	0.4685 (3)	0.45184 (8)	0.0536 (6)
O3	0.24162 (13)	0.8728 (4)	0.27949 (11)	0.0837 (9)
O4	0.20263 (9)	0.6294 (2)	0.30835 (7)	0.0441 (5)
O5	0.18423 (11)	0.8918 (3)	0.39870 (10)	0.0624 (7)
O6	0.24504 (12)	1.1218 (3)	0.38462 (13)	0.0812 (9)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.056 (3)	0.201 (6)	0.087 (3)	0.026 (3)	−0.002 (2)	0.011 (4)
C2	0.056 (2)	0.072 (2)	0.055 (2)	0.0107 (17)	−0.0103 (16)	−0.0021 (17)
C3	0.0484 (18)	0.071 (2)	0.0370 (16)	0.0034 (15)	0.0055 (13)	−0.0026 (15)
C4	0.0529 (18)	0.0413 (15)	0.0428 (16)	0.0034 (13)	−0.0097 (14)	−0.0052 (13)
C5	0.0364 (16)	0.0516 (17)	0.0405 (15)	−0.0100 (13)	−0.0011 (12)	0.0145 (13)
C6	0.0384 (15)	0.0360 (14)	0.0377 (15)	−0.0082 (12)	−0.0034 (12)	0.0062 (12)
C7	0.0345 (14)	0.0342 (13)	0.0344 (14)	−0.0035 (11)	−0.0032 (11)	0.0034 (11)
C8	0.0417 (16)	0.0445 (16)	0.0384 (15)	−0.0039 (13)	−0.0077 (12)	0.0089 (13)
C9	0.0371 (16)	0.0630 (19)	0.0566 (19)	0.0025 (14)	−0.0149 (14)	−0.0001 (15)
C10	0.048 (2)	0.103 (3)	0.102 (3)	−0.021 (2)	−0.016 (2)	0.015 (3)
C11	0.0331 (14)	0.0333 (13)	0.0424 (15)	−0.0056 (11)	−0.0004 (11)	0.0038 (11)
C12	0.0420 (17)	0.0380 (15)	0.0581 (19)	−0.0074 (13)	−0.0053 (14)	−0.0002 (13)
C13	0.080 (3)	0.068 (3)	0.124 (4)	0.010 (2)	−0.005 (3)	0.018 (3)
C14	0.127 (5)	0.117 (4)	0.140 (5)	0.008 (4)	0.030 (4)	−0.047 (4)
C15	0.0483 (18)	0.0383 (15)	0.0544 (18)	−0.0111 (13)	−0.0062 (14)	−0.0022 (13)
C16	0.0562 (19)	0.0498 (17)	0.0351 (15)	−0.0069 (14)	0.0009 (13)	−0.0058 (13)
C17	0.0535 (19)	0.0525 (18)	0.0559 (19)	−0.0064 (15)	−0.0116 (15)	−0.0058 (15)
C18	0.070 (2)	0.074 (2)	0.081 (3)	−0.010 (2)	−0.026 (2)	0.017 (2)
N1	0.0513 (16)	0.0541 (15)	0.0435 (14)	0.0085 (12)	−0.0034 (12)	−0.0020 (12)

N2	0.0381 (13)	0.0480 (13)	0.0356 (12)	−0.0042 (10)	−0.0001 (10)	0.0049 (10)
N3	0.0406 (13)	0.0338 (11)	0.0327 (12)	−0.0043 (9)	−0.0064 (9)	0.0023 (9)
N4	0.0376 (13)	0.0367 (12)	0.0433 (13)	−0.0089 (10)	−0.0043 (10)	0.0037 (10)
N5	0.0426 (13)	0.0362 (12)	0.0330 (12)	−0.0069 (10)	0.0022 (10)	0.0020 (9)
N6	0.0536 (15)	0.0437 (13)	0.0428 (14)	−0.0072 (12)	−0.0069 (11)	−0.0048 (11)
O1	0.0419 (13)	0.0848 (17)	0.0644 (15)	−0.0225 (12)	0.0067 (11)	0.0081 (12)
O2	0.0770 (16)	0.0419 (11)	0.0411 (11)	−0.0071 (10)	−0.0120 (10)	0.0114 (9)
O3	0.0736 (17)	0.0874 (18)	0.0875 (19)	−0.0298 (14)	−0.0399 (15)	0.0500 (16)
O4	0.0349 (11)	0.0496 (11)	0.0471 (12)	−0.0065 (9)	−0.0091 (9)	0.0052 (9)
O5	0.0426 (13)	0.0577 (14)	0.0871 (18)	−0.0013 (11)	0.0073 (12)	0.0011 (12)
O6	0.0559 (15)	0.0467 (14)	0.140 (3)	0.0042 (11)	−0.0048 (16)	0.0078 (15)

Geometric parameters (Å, °)

C1—C2	1.479 (6)	C10—H10A	0.9600
C1—H1A	0.9600	C10—H10B	0.9600
C1—H1B	0.9600	C10—H10C	0.9600
C1—H1C	0.9600	C11—N5	1.448 (3)
C2—N1	1.469 (4)	C11—N4	1.449 (3)
C2—H2A	0.9700	C11—C12	1.544 (4)
C2—H2B	0.9700	C12—O5	1.192 (3)
C3—N1	1.446 (4)	C12—O6	1.302 (4)
C3—N2	1.475 (4)	C13—C14	1.438 (7)
C3—H3A	0.9700	C13—O6	1.485 (5)
C3—H3B	0.9700	C13—H13A	0.9700
C4—N1	1.448 (4)	C13—H13B	0.9700
C4—N3	1.468 (4)	C14—H14A	0.9600
C4—H4A	0.9700	C14—H14B	0.9600
C4—H4B	0.9700	C14—H14C	0.9600
C5—O1	1.212 (3)	C15—N6	1.452 (4)
C5—N2	1.377 (4)	C15—N4	1.474 (4)
C5—N4	1.386 (4)	C15—H15A	0.9700
C6—O2	1.210 (3)	C15—H15B	0.9700
C6—N5	1.377 (3)	C16—N6	1.448 (4)
C6—N3	1.388 (3)	C16—N5	1.469 (3)
C7—N2	1.442 (3)	C16—H16A	0.9700
C7—N3	1.444 (3)	C16—H16B	0.9700
C7—C8	1.547 (4)	C17—N6	1.471 (4)
C7—C11	1.564 (4)	C17—C18	1.506 (5)
C8—O3	1.192 (3)	C17—H17A	0.9700
C8—O4	1.293 (3)	C17—H17B	0.9700
C9—O4	1.460 (3)	C18—H18A	0.9600
C9—C10	1.464 (5)	C18—H18B	0.9600
C9—H9A	0.9700	C18—H18C	0.9600
C9—H9B	0.9700		
C2—C1—H1A	109.5	O5—C12—C11	120.7 (3)
C2—C1—H1B	109.5	O6—C12—C11	112.4 (3)
H1A—C1—H1B	109.5	C14—C13—O6	108.3 (5)
C2—C1—H1C	109.5	C14—C13—H13A	110.0

H1A—C1—H1C	109.5	O6—C13—H13A	110.0
H1B—C1—H1C	109.5	C14—C13—H13B	110.0
N1—C2—C1	113.3 (3)	O6—C13—H13B	110.0
N1—C2—H2A	108.9	H13A—C13—H13B	108.4
C1—C2—H2A	108.9	C13—C14—H14A	109.5
N1—C2—H2B	108.9	C13—C14—H14B	109.5
C1—C2—H2B	108.9	H14A—C14—H14B	109.5
H2A—C2—H2B	107.7	C13—C14—H14C	109.5
N1—C3—N2	113.8 (2)	H14A—C14—H14C	109.5
N1—C3—H3A	108.8	H14B—C14—H14C	109.5
N2—C3—H3A	108.8	N6—C15—N4	113.7 (2)
N1—C3—H3B	108.8	N6—C15—H15A	108.8
N2—C3—H3B	108.8	N4—C15—H15A	108.8
H3A—C3—H3B	107.7	N6—C15—H15B	108.8
N1—C4—N3	113.4 (2)	N4—C15—H15B	108.8
N1—C4—H4A	108.9	H15A—C15—H15B	107.7
N3—C4—H4A	108.9	N6—C16—N5	113.3 (2)
N1—C4—H4B	108.9	N6—C16—H16A	108.9
N3—C4—H4B	108.9	N5—C16—H16A	108.9
H4A—C4—H4B	107.7	N6—C16—H16B	108.9
O1—C5—N2	125.9 (3)	N5—C16—H16B	108.9
O1—C5—N4	125.8 (3)	H16A—C16—H16B	107.7
N2—C5—N4	108.2 (2)	N6—C17—C18	111.9 (3)
O2—C6—N5	125.9 (3)	N6—C17—H17A	109.2
O2—C6—N3	125.9 (3)	C18—C17—H17A	109.2
N5—C6—N3	108.1 (2)	N6—C17—H17B	109.2
N2—C7—N3	111.5 (2)	C18—C17—H17B	109.2
N2—C7—C8	110.0 (2)	H17A—C17—H17B	107.9
N3—C7—C8	114.1 (2)	C17—C18—H18A	109.5
N2—C7—C11	103.2 (2)	C17—C18—H18B	109.5
N3—C7—C11	103.9 (2)	H18A—C18—H18B	109.5
C8—C7—C11	113.6 (2)	C17—C18—H18C	109.5
O3—C8—O4	126.2 (3)	H18A—C18—H18C	109.5
O3—C8—C7	120.0 (3)	H18B—C18—H18C	109.5
O4—C8—C7	113.7 (2)	C3—N1—C4	110.5 (2)
O4—C9—C10	108.1 (3)	C3—N1—C2	115.3 (3)
O4—C9—H9A	110.1	C4—N1—C2	113.4 (3)
C10—C9—H9A	110.1	C5—N2—C7	111.8 (2)
O4—C9—H9B	110.1	C5—N2—C3	124.1 (2)
C10—C9—H9B	110.1	C7—N2—C3	114.9 (2)
H9A—C9—H9B	108.4	C6—N3—C7	110.9 (2)
C9—C10—H10A	109.5	C6—N3—C4	123.2 (2)
C9—C10—H10B	109.5	C7—N3—C4	115.5 (2)
H10A—C10—H10B	109.5	C5—N4—C11	110.7 (2)
C9—C10—H10C	109.5	C5—N4—C15	121.9 (2)
H10A—C10—H10C	109.5	C11—N4—C15	115.6 (2)
H10B—C10—H10C	109.5	C6—N5—C11	111.7 (2)
N5—C11—N4	111.7 (2)	C6—N5—C16	123.5 (2)
N5—C11—C12	109.6 (2)	C11—N5—C16	115.2 (2)

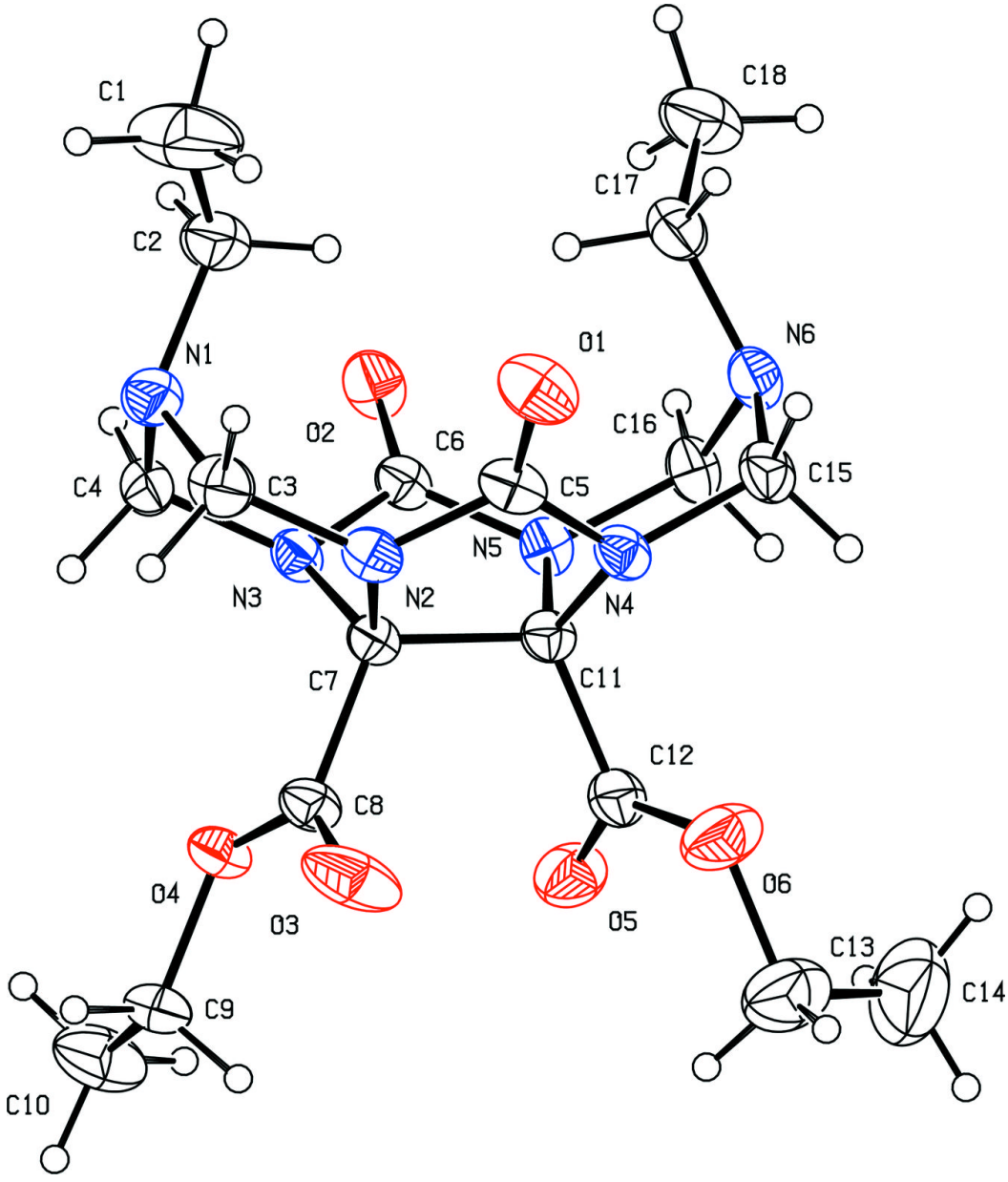
N4—C11—C12	114.4 (2)	C16—N6—C15	110.0 (2)
N5—C11—C7	103.1 (2)	C16—N6—C17	114.5 (2)
N4—C11—C7	103.7 (2)	C15—N6—C17	114.0 (3)
C12—C11—C7	113.6 (2)	C8—O4—C9	116.6 (2)
O5—C12—O6	126.8 (3)	C12—O6—C13	116.6 (3)
N2—C7—C8—O3	−44.8 (4)	C8—C7—N3—C6	−134.4 (2)
N3—C7—C8—O3	−170.9 (3)	C11—C7—N3—C6	−10.2 (3)
C11—C7—C8—O3	70.3 (4)	N2—C7—N3—C4	−46.0 (3)
N2—C7—C8—O4	138.7 (2)	C8—C7—N3—C4	79.3 (3)
N3—C7—C8—O4	12.6 (3)	C11—C7—N3—C4	−156.5 (2)
C11—C7—C8—O4	−106.1 (3)	N1—C4—N3—C6	−91.5 (3)
N2—C7—C11—N5	−115.2 (2)	N1—C4—N3—C7	50.3 (3)
N3—C7—C11—N5	1.2 (2)	O1—C5—N4—C11	−166.8 (3)
C8—C7—C11—N5	125.7 (2)	N2—C5—N4—C11	15.9 (3)
N2—C7—C11—N4	1.4 (2)	O1—C5—N4—C15	−25.8 (4)
N3—C7—C11—N4	117.8 (2)	N2—C5—N4—C15	156.9 (2)
C8—C7—C11—N4	−117.7 (2)	N5—C11—N4—C5	100.0 (3)
N2—C7—C11—C12	126.2 (2)	C12—C11—N4—C5	−134.7 (2)
N3—C7—C11—C12	−117.4 (2)	C7—C11—N4—C5	−10.4 (3)
C8—C7—C11—C12	7.1 (3)	N5—C11—N4—C15	−43.7 (3)
N5—C11—C12—O5	−50.3 (4)	C12—C11—N4—C15	81.6 (3)
N4—C11—C12—O5	−176.7 (3)	C7—C11—N4—C15	−154.1 (2)
C7—C11—C12—O5	64.4 (4)	N6—C15—N4—C5	−90.4 (3)
N5—C11—C12—O6	132.3 (3)	N6—C15—N4—C11	49.0 (3)
N4—C11—C12—O6	6.0 (4)	O2—C6—N5—C11	168.3 (3)
C7—C11—C12—O6	−112.9 (3)	N3—C6—N5—C11	−15.0 (3)
N2—C3—N1—C4	51.4 (3)	O2—C6—N5—C16	24.0 (4)
N2—C3—N1—C2	−78.8 (3)	N3—C6—N5—C16	−159.4 (2)
N3—C4—N1—C3	−51.2 (3)	N4—C11—N5—C6	−102.5 (3)
N3—C4—N1—C2	79.9 (3)	C12—C11—N5—C6	129.5 (2)
C1—C2—N1—C3	−65.4 (5)	C7—C11—N5—C6	8.2 (3)
C1—C2—N1—C4	165.8 (4)	N4—C11—N5—C16	44.9 (3)
O1—C5—N2—C7	167.7 (3)	C12—C11—N5—C16	−83.0 (3)
N4—C5—N2—C7	−15.1 (3)	C7—C11—N5—C16	155.7 (2)
O1—C5—N2—C3	22.6 (4)	N6—C16—N5—C6	91.7 (3)
N4—C5—N2—C3	−160.1 (2)	N6—C16—N5—C11	−51.5 (3)
N3—C7—N2—C5	−102.8 (3)	N5—C16—N6—C15	53.3 (3)
C8—C7—N2—C5	129.7 (2)	N5—C16—N6—C17	−76.6 (3)
C11—C7—N2—C5	8.1 (3)	N4—C15—N6—C16	−52.1 (3)
N3—C7—N2—C3	45.7 (3)	N4—C15—N6—C17	78.1 (3)
C8—C7—N2—C3	−81.9 (3)	C18—C17—N6—C16	−66.0 (3)
C11—C7—N2—C3	156.6 (2)	C18—C17—N6—C15	166.1 (3)
N1—C3—N2—C5	93.8 (3)	O3—C8—O4—C9	2.6 (5)
N1—C3—N2—C7	−50.3 (3)	C7—C8—O4—C9	178.8 (2)
O2—C6—N3—C7	−167.5 (3)	C10—C9—O4—C8	−162.9 (3)
N5—C6—N3—C7	15.8 (3)	O5—C12—O6—C13	−1.5 (6)
O2—C6—N3—C4	−24.3 (4)	C11—C12—O6—C13	175.7 (3)
N5—C6—N3—C4	159.1 (2)	C14—C13—O6—C12	83.9 (5)
N2—C7—N3—C6	100.3 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4B···O3^{i}	0.97	2.53	3.460 (4)	160

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

Fig. 1


C1
C2
N1
C4
C3
N3
O2
C6
N2
C7
C8
O4
O3
C9
C10
O1
C5
N5
N4
C11
C12
O5
O6
C13
C14
C18
C17
N6
C16
C15