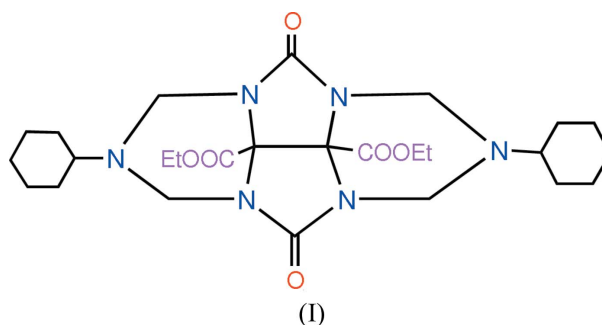


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Key indicators

Single-crystal X-ray study
 $T = 292$ K
Mean $\sigma(\text{C}-\text{C}) = 0.006$ Å
 R factor = 0.065
 wR factor = 0.188
Data-to-parameter ratio = 13.6For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Diethyl 2,6-dicyclohexyl-4,8-dioxo-2,2,3,6,7-
tetrahydro-1*H*,5*H*-2,3*a*,4*a*,6,7*a*,8*a*-hexaaza-
cyclopenta[*def*]fluorene-8*b*,8*c*-dicarboxylateIn the title compound, $\text{C}_{26}\text{H}_{40}\text{N}_6\text{O}_6$, the five-membered rings
adopt envelope conformations and the six-membered rings
are in chair conformations. The crystal packing is stabilized by
 $\text{C}-\text{H} \cdots \text{O}$ hydrogen bonds.Received 23 August 2005
Accepted 16 September 2005
Online 21 September 2005

Comment

In current coordination and supramolecular chemistry, the
rational design of coordination architectures represents one of
the most exciting and rapidly developing fields, owing to their
potential as functional materials (Braga *et al.*, 1998). Glyco-
luril derivatives have applications in many areas, such as
explosives, slow-release fertilizers, crosslinkers, iodogens,
stabilizers of organic compounds against photodegradation,
and reagents in combinatorial chemistry (Wu *et al.*, 2002).
Here we report the structure of the title compound, (I)
(Fig. 1), as a continuation of our previous studies in this area
(Li & Wu, 2005).The molecule of (I) exhibits normal geometric parameters
(Table 1), except for shortened $\text{C}-\text{C}$ distances in the ethyl
groups. The imidazolidine rings adopt envelope conforma-
tions, whereas the cyclohexane and triazinane rings are in
chair conformations. The crystal packing is stabilized by $\text{C}-$
 $\text{H} \cdots \text{O}$ hydrogen bonds (Fig. 2 and Table 2).

Experimental

Cyclohexylamine (0.99 g, 10 mmol) and formaldehyde (1.2 g,
40 mmol) were added to a stirred solution of diethyl 2,5-dioxotetra-
hydroimidazo[4,5-*d*]imidazole-3*a*,6*a*-dicarboxylate (1.43 g, 5 mmol)
in acetonitrile (50 ml) under a nitrogen atmosphere. The mixture was
stirred overnight at room temperature. The solvent was evaporated
and the compound was purified by column chromatography to yield
(I) (2.40 g, 90%) as a colourless solid. Colourless block-like crystals
of (I) suitable for X-ray data collection were obtained by slow
evaporation of an acetic acid–ethyl acetate solution at 283 K.

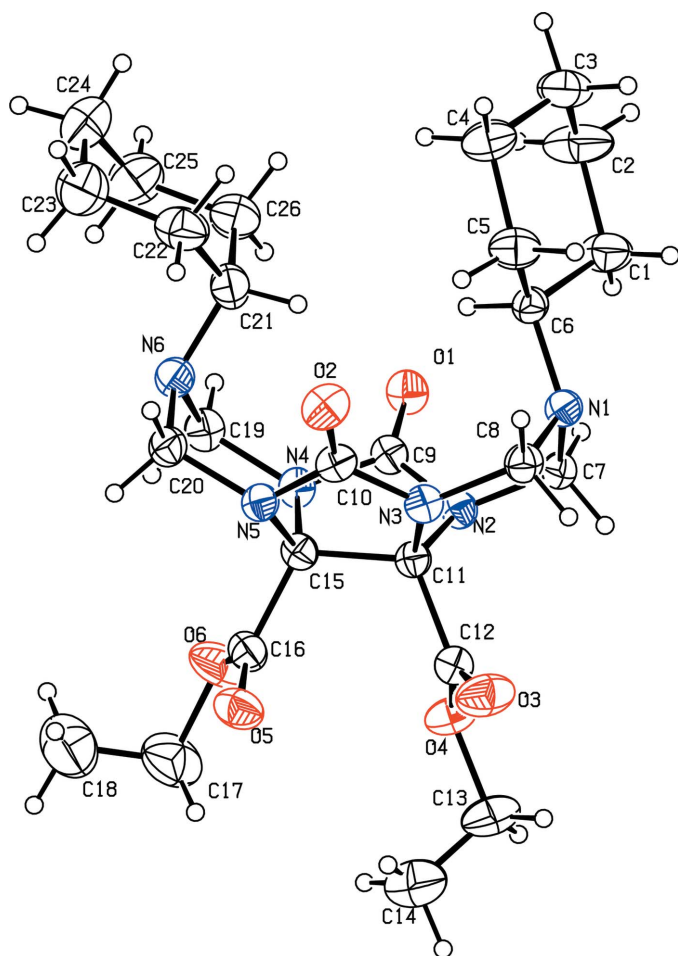


Figure 1
A view of the molecule of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

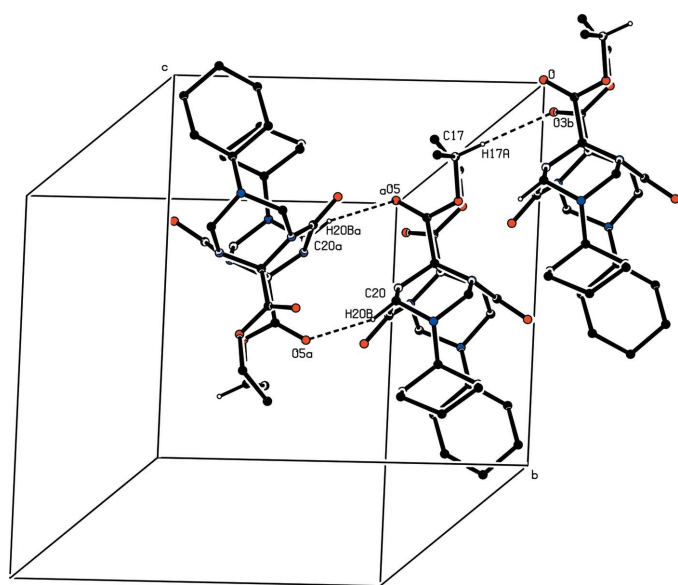


Figure 2
Part of the crystal packing of (I). Dashed lines indicate hydrogen bonds. Atoms labeled with the suffixes a and b are generated by the symmetry codes $(-x, 1-y, 1-z)$ and $(x-1, y, z)$, respectively.

Crystal data

$C_{26}H_{40}N_6O_6$
 $M_r = 532.64$
 Triclinic, $P\bar{1}$
 $a = 7.9337$ (8) Å
 $b = 13.0996$ (13) Å
 $c = 13.9361$ (14) Å
 $\alpha = 78.913$ (2)°
 $\beta = 79.686$ (2)°
 $\gamma = 74.259$ (2)°
 $V = 1355.6$ (2) Å³

$Z = 2$
 $D_x = 1.305$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 1576 reflections
 $\theta = 2.4$ – 21.5 °
 $\mu = 0.09$ mm⁻¹
 $T = 292$ (2) K
 Block, colorless
 $0.40 \times 0.18 \times 0.08$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1997)
 $T_{\min} = 0.963$, $T_{\max} = 0.993$
 6851 measured reflections

4685 independent reflections
 3120 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.022$
 $\theta_{\text{max}} = 25.0$ °
 $h = -9 \rightarrow 9$
 $k = -15 \rightarrow 15$
 $l = -16 \rightarrow 8$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.065$
 $wR(F^2) = 0.188$
 $S = 1.05$
 4685 reflections
 345 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0926P)^2 + 0.2271P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.36$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.29$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

C1–C6	1.504 (4)	C10–O2	1.209 (3)
C6–N1	1.482 (3)	C10–N3	1.370 (4)
C7–N1	1.456 (3)	C11–N3	1.443 (3)
C8–N1	1.452 (3)	C11–C12	1.546 (4)
C9–O1	1.212 (3)	C12–O3	1.186 (3)
C9–N2	1.393 (3)	C13–C14	1.407 (7)
N1–C6–C1	108.6 (2)	O3–C12–O4	125.5 (3)
C1–C6–C5	109.6 (2)	O4–C12–C11	111.0 (2)
N1–C7–N2	113.6 (2)	O5–C16–O6	126.5 (3)
N1–C8–N3	113.3 (2)	O6–C16–C15	112.1 (3)
N3–C11–C12–O3	2.8 (4)	C12–C11–C15–N5	113.4 (2)
C15–C11–C12–O3	–113.6 (3)	N3–C11–C15–C16	–125.9 (2)
N3–C11–C12–O4	–176.0 (2)	C12–C11–C15–C16	–6.0 (3)
C15–C11–C12–O4	67.6 (3)	N4–C15–C16–O5	–175.3 (3)
N3–C11–C15–N4	109.9 (2)	C11–C15–C16–O5	66.8 (3)
C12–C11–C15–N4	–130.2 (2)	N4–C15–C16–O6	7.0 (3)
N3–C11–C15–N5	–6.5 (2)	C11–C15–C16–O6	–110.9 (3)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C20–H20B ⁱ ⋯O5 ⁱ	0.97	2.49	3.381 (4)	152
C17–H17A ⁱⁱ ⋯O3 ⁱⁱ	0.97	2.55	3.513 (6)	171

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $x-1, y, z$.

Methyl H atoms were constrained to an ideal geometry, with $C-H = 0.96$ Å and $U_{\text{iso}}(H) = 1.5U_{\text{eq}}(C)$, but each group was allowed to rotate freely about its $C-C$ bond. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with $C-H = 0.97$ or 0.98 Å and $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$.

As attempts to restrain the C13—C14 and C17—C18 bond distances of the ethyl groups to 1.53 (1) Å resulted in limited improvement [1.444 (6) and 1.450 (6) Å, respectively], the restraints were not used. Also, no suitable disorder model was found for the ethyl groups.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINTE* (Bruker, 2000); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

The authors are grateful to the Central China Normal University, the National Natural Science Foundation of China

(grant No. 20472022) and the Hubei Province Natural Science Fund (grant Nos. 2004ABA085 and 2004ABC002) for financial support.

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