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2,6-Dibenzhydryl-8b,8c-diphenyl-2,3,5,6,8b,8c-hexahydro-2,3a,4a,6,7a,8a-hexaaza-1*H*,4*H*-cyclopenta[*def*]fluorene-4,8-dione

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.007 Å
R factor = 0.064
wR factor = 0.190
Data-to-parameter ratio = 13.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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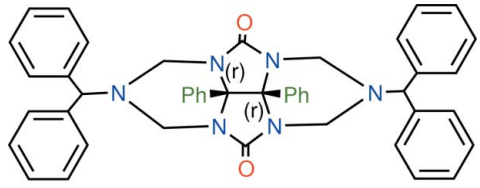
The title compound, $C_{46}H_{40}N_6O_2$, is a glycoluril derivative. The molecule contains four fused rings, *viz* two nearly planar imidazole rings and two non-planar triazine rings. The triazine rings each have a chair conformation.

Comment

Glycoluril derivatives have many areas of applications, such as explosives, slow-release fertilizers, cross-linkers, iodogens, stabilizers of organic compounds against photodegradation, and as reagents in combinatorial chemistry (Wu *et al.*, 2002). As a continuation of our previous studies in this area (Wei & Wu, 2005), we present here the structure of the title compound, (I).



(I)

The molecular structure of (I) is shown in Fig. 1. The molecule contains four fused rings, *viz*. two nearly planar imidazole rings and two non-planar triazine rings. The non-planar six-membered rings display chair conformations, as observed in the related compound dimethyl 2,6-di-*tert*-butyl-4,8-dioxo-1,2,5,6-tetrahydro-2,3a,4a,6,7a,8a-hexaazacyclopenta[*def*]-

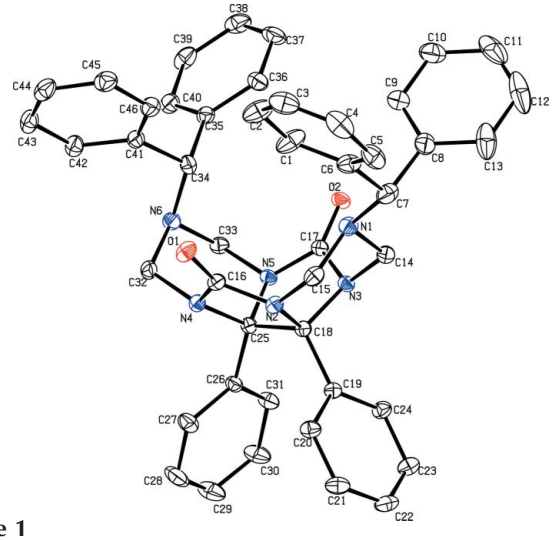


Figure 1
A view of the molecule of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted.

fluorene-8b,8c-dicarboxylate (Li *et al.*, 2005). All distances and angles are normal within experimental error.

Experimental

C,*C*-Diphenylmethylamine (1.83 g, 10 mmol) and formaldehyde (2.4 g, 40 mmol) were added to a stirred solution of 3a,6a-diphenyltetrahydroimidazo[4,5-*d*]imidazole-2,5-dione (1.47 g, 5 mmol) in acetonitrile (50 ml) under a nitrogen atmosphere. The mixture was stirred overnight at room temperature. The solvent was evaporated to dryness and the residue was purified by column chromatography, yielding (I) (3.18 g, 90%) as a colorless solid. Colorless block-like crystals of (I) suitable for data collection were obtained by slow evaporation of an ethyl acetate solution at 283 K.

Crystal data

$C_{46}H_{40}N_6O_2$	$Z = 2$
$M_r = 708.84$	$D_x = 1.238$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 10.5691$ (13) Å	Cell parameters from 2204 reflections
$b = 13.7434$ (17) Å	$\theta = 2.5$–$21.4°$
$c = 13.9871$ (17) Å	$\mu = 0.08$ mm^{-1}
$\alpha = 78.876$ (2)°	$T = 292$ (2) K
$\beta = 72.706$ (2)°	Block, colorless
$\gamma = 88.624$ (2)°	0.30 × 0.20 × 0.20 mm
$V = 1902.2$ (4) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	3963 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.018$
Absorption correction: none	$\theta_{max} = 25.0°$
9562 measured reflections	$h = -12 \rightarrow 12$
6617 independent reflections	$k = -16 \rightarrow 16$
	$l = -8 \rightarrow 16$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0818P)^2 + 0.5417P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.064$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.190$	$\Delta\rho_{max} = 0.32$ e Å^{-3}
$S = 1.03$	$\Delta\rho_{min} = -0.18$ e Å^{-3}
6617 reflections	
487 parameters	
H-atom parameters constrained	

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.98 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ or $U_{iso}(H) = 1.5U_{eq}(C)$.

Data collection: *SMART* (Bruker,2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; 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*.

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