Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

1,1′,3,3′-Tetrabenzyl-2,2′-biimidazolidine

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.048
wR factor = 0.140
Data-to-parameter ratio = 18.5

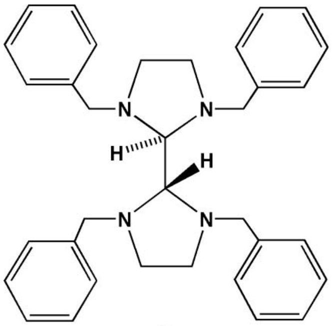
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 16 June 2005
Accepted 4 July 2005
Online 9 July 2005

The title compound, $C_{34}H_{38}N_4$, possesses C_i symmetry. The supramolecular structure is achieved by intramolecular C—H···N and weak intermolecular C—H···π interactions.

Comment

The reaction of primary amines (RNH_2) with glyoxal gives a variety of products depending on the nature of the amine and, in certain cases, the reaction conditions (Willer *et al.*, 1985; Koppes *et al.*, 1987). Some biimidazolidine derivatives such as enetetramines have been extensively studied (Hoffmann, 1968; Hocker & Merten, 1972; Roeterdink *et al.*, 1983).



(I)

In the centrosymmetric title compound, (I), each N atom has a pyramidal configuration and is substituted with a benzyl group (Fig. 1). The bond angles around the N atoms (Table 1) are in the range reported for bond angles in similar biimidazolidine derivatives, such as 1,3,1′,3′-tetrabenzyl-2–2′-biimidazolidinylidenes and hexaazaisowurtzitanes [N—C—N = 101.3 (3)–120.2 (4)° and C—N—C = 102.2 (3)–114.6 (4)°; Cetinkaya *et al.*, 1998; Klapötke *et al.*, 2003]. The heterocyclic ring has a half-chair conformation. The bond lengths C3—C3^{i}, N1—C1, N1—C3, N1—C11, N2—C2, N2—C3 and N2—C4 (see Table 1 for bond lengths and symmetry code) are characteristic for Csp^3—Csp^3 and Csp^3—N (Nsp^3: pyramidal) (Allen *et al.*, 1987). The molecule shows an intramolecular C4—H4*B*···N1 hydrogen bond (Table 2). The supramolecular structure, shown in Fig. 2, is achieved by weak intermolecular C—H···π interactions (Table 2).

Experimental

The title compound was prepared from *N*,*N*-dibenzylethylenediamine and glyoxal [m.p. 404 K; literature 403 K (Willer *et al.*, 1985)]. Single crystals suitable for X-ray diffraction were grown from an acetonitrile solution at room temperature by slow evaporation.

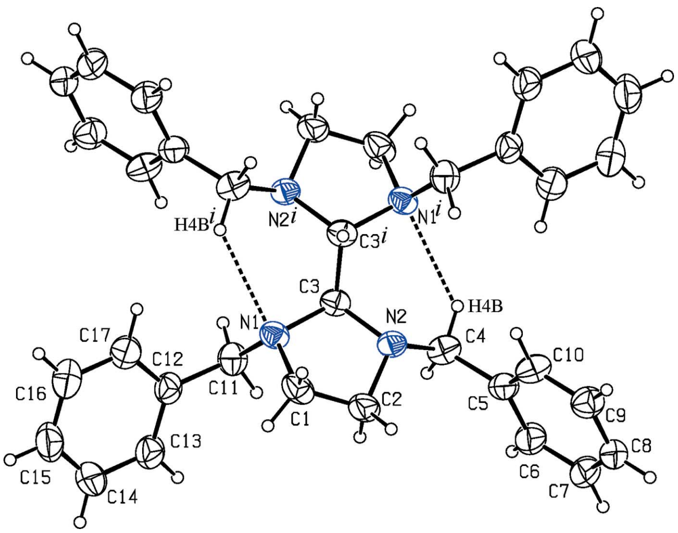


Figure 1
View of (I), with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Dashed lines indicate intramolecular N—H···N hydrogen bonds [symmetry code: (i) 2 − *x*, 1 − *y*, −*z*].

Crystal data

$C_{34}H_{38}N_4$
M_r = 502.68
Monoclinic, $P2_1/c$
a = 5.8384 (1) Å
b = 9.6253 (2) Å
c = 25.7216 (4) Å
β = 93.4210 (10)°
V = 1442.88 (4) Å^3
Z = 2
D_x = 1.157 Mg m^{-3}
Mo *K*α radiation
Cell parameters from 600 reflections
θ = 20–25°
μ = 0.07 mm^{-1}
T = 293 (2) K
Block, colorless
0.15 × 0.1 × 0.09 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: none
4969 measured reflections
3185 independent reflections
2262 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 27.5°
h = −7 → 7
k = −12 → 8
l = −33 → 33

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.140
S = 1.03
3185 reflections
172 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0668P)^2 + 0.1647P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—C1	1.4751 (18)	N2—C2	1.4555 (18)
N1—C3	1.4765 (16)	N2—C3	1.4845 (16)
N1—C11	1.4630 (18)	N2—C4	1.4607 (17)
C1—N1—C3	104.62 (10)	N2—C2—C1	102.27 (11)
C1—N1—C11	112.90 (11)	N1—C3—N2	107.16 (10)
C3—N1—C11	112.84 (11)	N1—C3—C3^i	111.00 (10)
C2—N2—C3	106.37 (10)	N2—C3—C3^i	109.96 (10)
C2—N2—C4	113.03 (11)	N2—C4—C5	112.08 (10)
C3—N2—C4	113.73 (10)	N1—C11—C12	112.39 (13)
N1—C1—C2	105.16 (12)		

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

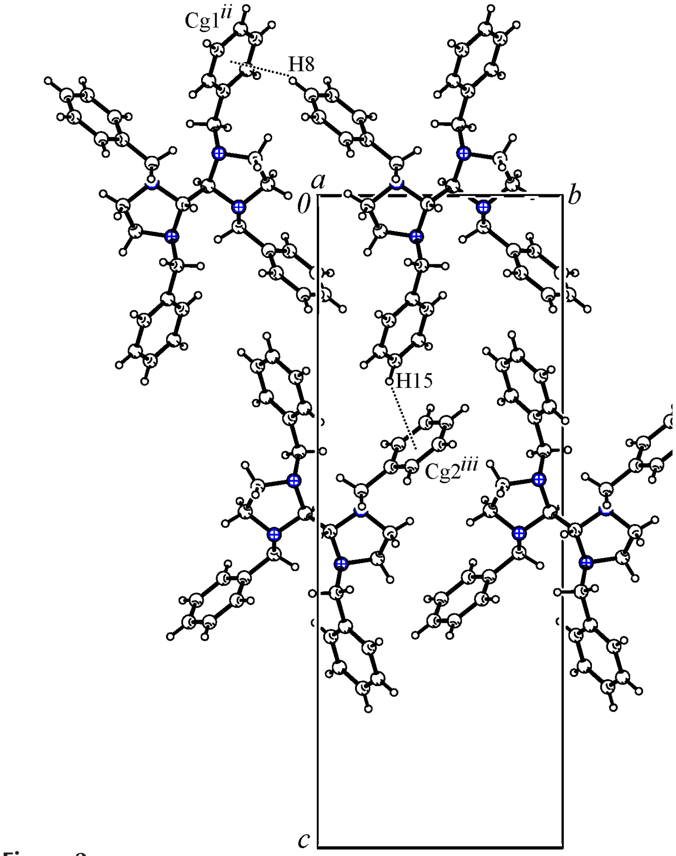


Figure 2
The supramolecular structure of (I), viewed along the *a* axis [symmetry codes: (ii) 2 − *x*, −*y*, −*z*; (iii) 1 + *x*, $\frac{1}{2}$ − *y*, $\frac{1}{2}$ + *z*].

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4*B*···N1^i	0.97	2.58	3.2011 (17)	122
C8—H8···*Cg*1^{ii}	0.93	3.07	3.8140 (18)	139
C15—H15···*Cg*2^{iii}	0.93	3.10	3.894 (2)	144

Symmetry codes: (i) $-x+2, -y+1, -z$; (ii) $-x+2, -y, -z$; (iii) $x+1, -y+\frac{1}{2}, +z+\frac{1}{2}$. *Cg*1 and *Cg*2 are the controids of benzene rings, C5–C10 and C12–C17, respectively

All H atoms were placed at calculated positions and refined using a riding model, with C—H = 0.93 or 0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick 1997); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors thank the Consejo Superior de la Investigación Científica in Spain for the award of a license for the use of the Cambridge Crystallographic Database (Allen, 2002).

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Acta Cryst. (2005). E**61**, o2464–o2466 López *et al.* • $C_{34}H_{38}N_4$ **o2465**

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