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1,4-Bis(benzimidazol-2-yl)butane

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.039
wR factor = 0.106
Data-to-parameter ratio = 16.1

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

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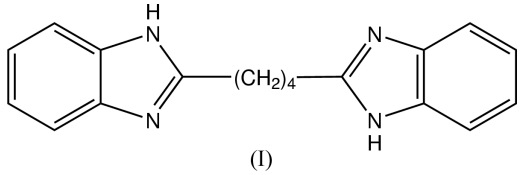
The title compound, $C_{18}H_{18}N_4$, lies on an inversion center. The benzimidazolyl moiety is essentially planar. Intermolecular N—H···N hydrogen bonds give rise to an infinite helical chain structure, with the chains stacked by C—H···π and π···π interactions.

Comment

Since it was found that imidazole is a component of biologically important molecules (Reedijk, 1987), the coordination chemistry of related ligand has been the subject of numerous investigations (Reedijk, 1987) and has attracted much interest in the past decades. In this respect, bis(benzimidazol-2-yl)-substituted compounds have received much attention for their wide-ranging antiviral activity (Tidwell *et al.*, 1993), photochemical and photophysical properties (Santra & Dogra, 1999), their importance in selective ion-exchange resins (Albada *et al.*, 2002), and the possibility to form supramolecular aggregates with transition metal ions (Su *et al.*, 2001; Vaidyanathan *et al.*, 2001). In the meanwhile, weak interactions, such as N—H···N and π···π, between benzimidazole rings are of interest to chemists in the construction of new complexes (Yang *et al.*, 2000; Nishida & Takahashi, 1998; Unamuno *et al.*, 1998). Here we report the crystal and molecular structure of the title compound, (I).



(I)

The stepped molecule lies on an inversion center at the midpoint of C9—C9*A*(1 − *x*, 1 − *y*, − *z*) (Fig. 1). The C7—C8, C8—C9, C9—C9*A* bond lengths are all close to the standard value for a single-bond length. The average bond distances and angles for the benzimidazole ring are in agreement with those of other bis(benzimidazolyl)-substituted compounds (Matthews *et al.*, 1996; Ozbey *et al.*, 1998). The C—N bond lengths in the imidazole ring are in the range 1.3112 (17)–1.3900 (16) Å; these are shorter than the single-bond length of 1.480 Å and longer than the typical C═N distance of 1.280 Å, indicating partial double-bond character. This can be interpreted in terms of conjugation in the heterocycle; the dihedral angle between the six- and five-membered rings is only 1.63 (11)°, showing almost exact coplanarity. The molecules form a two-dimensional network through intermolecular N—H···N hydrogen bonds, and C—H···π and π···π interactions. The hydrogen-bonded helical chains, parallel to *b*, are stacked upon one another by translation and held together by C—H···π and π···π interactions.

Experimental

The title compound was prepared from hexanedioic acid and 1,2-diaminobenzene, in 63.38% yield, using a modified Phillips reaction (Addison & Burke, 1981; Addison *et al.*, 1983) and was recrystallized from EtOH. Single crystals suitable for X-ray analysis were then obtained by slow evaporation at room temperature from an EtOH solution.

Crystal data

$C_{18}H_{18}N_4$
$M_r = 290.36$
Orthorhombic, *Pbca*
$a = 8.793$ (5) Å
$b = 9.366$ (5) Å
$c = 17.881$ (10) Å
$V = 1472.6$ (14) Å^3
$Z = 4$
$D_x = 1.31$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4154 reflections
$\theta = 3.3$–27.2°
$\mu = 0.08$ mm^{-1}
$T = 293$ (2) K
Block, purple
0.50 × 0.30 × 0.27 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: empirical (Blessing, 1995)
$T_{min} = 0.897$, $T_{max} = 0.978$
7990 measured reflections
1614 independent reflections
1344 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$
$\theta_{max} = 27.2^\circ$
$h = -9 \rightarrow 11$
$k = -11 \rightarrow 11$
$l = -16 \rightarrow 22$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.106$
$S = 1.05$
1614 reflections
100 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.045P)^2 + 0.5071P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0$
$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—C1	1.3759 (17)	C3—C4	1.390 (2)
N1—C7	1.3573 (17)	C4—C5	1.378 (2)
N2—C7	1.3112 (17)	C5—C6	1.3880 (19)
N2—C6	1.3900 (16)	C7—C8	1.4871 (19)
C1—C6	1.3968 (19)	C8—C9	1.5185 (19)
C1—C2	1.3811 (18)	C9—C9^i	1.516 (3)
C2—C3	1.378 (2)		
C1—N1—C7	107.22 (10)	C7—N2—C6	105.04 (11)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···N2^i	0.86	2.21	3.0431 (19)	163

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

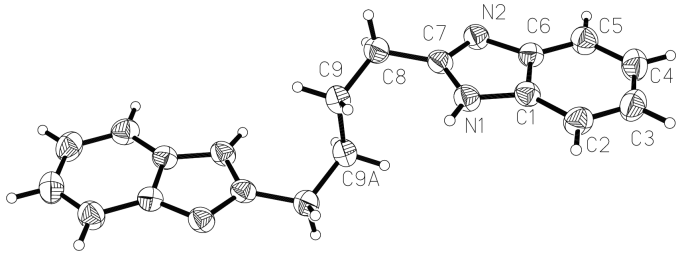


Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1999); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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