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N,*N*′-Bis(2-aminobenzyl)ethane-1,2-diamine

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Key indicators

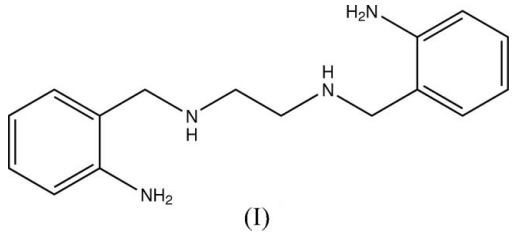
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.002 Å
R factor = 0.052
wR factor = 0.167
Data-to-parameter ratio = 16.0

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

The asymmetric unit of the title compound, $C_{16}H_{22}N_4$, contains one half of the molecule, which lies on a crystallographic inversion center.

Comment

The title compound, (I), a Schiff base ligand, has been synthesized as a chemical precursor for a variety of simple and macrocyclic multidentate ligands and metal complexes. Several crystal structures of complexes using (I) have been reported, with Cd^{II} (Ansell *et al.*, 1983), and with Ni^{II} (Anacona *et al.*, 2005; Taylor *et al.*, 2004).



(I)

Compound (I) crystallizes with the molecule lying on a crystallographic inversion center, located at the mid-point of the C8—C8^{i} bond [symmetry code: (i) $1-x$, $1-y$, $-z$] (Fig. 1). The conformation of the central chain is described by torsion angles C6—C7—N2—C8 = 175.26 (13)°, C7—N2—C8—C8^{i} = 81.3 (2)° and N2—C8—C8^{i}—N2^{i} constrained by symmetry to 180°. This *trans–gauche–trans* conformation stabilized in the solid state for (I) is less common than the all-*trans* conformation generally found in aliphatic systems. On the other hand, all the N atoms in (I) may coordinate to a metal center, giving another conformation for this ligand. These observations suggest that (I) is a highly flexible molecule, with almost free rotation about all σ bonds.

The molecule shows a weak intramolecular hydrogen bond involving N1 and N2 and an intermolecular contact formed between amine group N1 and a symmetry-related N2 group (Table 1), forming a chain along the *a* axis (Fig. 2). Finally, the H atom of the N2 amine group does not participate in any hydrogen bonds with a symmetry-related molecule. This preferential and more extended hydrogen-bonding formation, using the NH_2 substituents rather than the NH functionalities of the central diaminoethane group, probably gives a more stable crystal structure.

Experimental

Published procedures were used (Elizondo-Martínez *et al.*, 2006; Obregón-Solís *et al.*, 2001) to prepare *N*,*N*′-bis(2-nitrobenzyl)-1,2-

diaminoethane. A Pd/C-catalysed selective reduction reaction of this compound using $NH_2NH_2{\cdot}H_2O$ afforded (I) together with a 2*H*-indazole compound, [2,2′-(ethane-1,2-diyl)bis(2*H*-indazole)] (Rodríguez de Barbarín *et al.*, 2006). Suitable crystals were obtained as yellow prisms from ethanol by slow evaporation at 298 K. The solid was characterized by IR and ^{1}H NMR spectroscopy and elemental analysis, which are in agreement with the X-ray crystal structure.

Crystal data

$C_{16}H_{22}N_4$
M_r = 270.38
Orthorhombic, *Pccn*
a = 9.974 (3) Å
b = 22.729 (7) Å
c = 6.384 (2) Å
V = 1447.2 (8) Å^3
Z = 4
D_x = 1.241 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 (2) K
Prism, yellow
0.60 × 0.60 × 0.45 mm

Data collection

Bruker P4 diffractometer
ω scans
Absorption correction: none
3702 measured reflections
1661 independent reflections
1191 reflections with $I > 2\sigma(I)$
R_{int} = 0.062
θ_{max} = 27.5°
3 standard reflections
every 97 reflections
intensity decay: 3%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.167
S = 1.02
1661 reflections
104 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0954P)^2 + 0.1803P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Extinction correction: *SHELXTL-Plus*
Extinction coefficient: 0.060 (14)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*B*···N2	0.91 (2)	2.32 (2)	2.994 (2)	131.3 (17)
N1—H1*A*···N2^{i}	0.88 (2)	2.39 (2)	3.264 (2)	172.3 (16)

Symmetry code: (i) $-x+\frac{3}{2}, y, z+\frac{1}{2}$.

The atoms H1*A*, H1*B* and H2*A* bonded to N atoms were found in difference maps and refined isotropically with free coordinates. H atoms bonded to C atoms were included in calculated positions, and refined using the riding method, with C—H distances constrained to 0.93 (aromatic CH) and 0.97 Å (methylene CH_2) and U_{iso}(H) = 1.2U_{eq}(carrier C).

Data collection: *XSCANS* (Siemens, 1996); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXTL-Plus* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL-Plus*; molecular graphics: *SHELXTL-Plus* and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXTL-Plus*.

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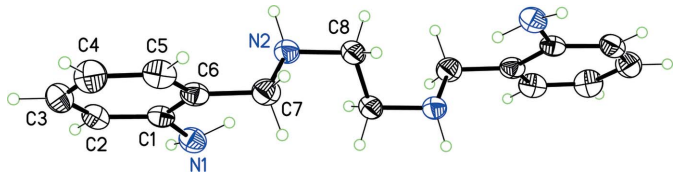

Figure 1
Molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radius. Unlabeled atoms are related to labeled atoms by (1 − x, 1 − y, −z).

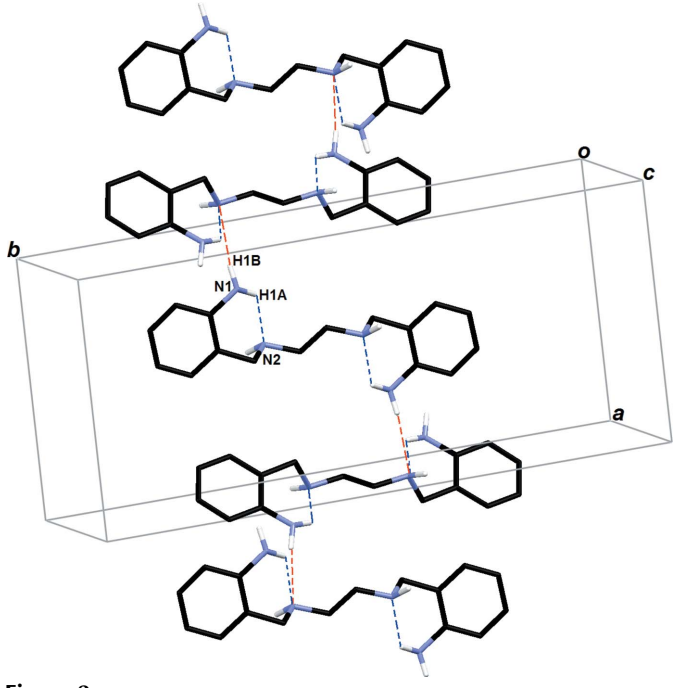

Figure 2
Molecular packing for (I), showing the hydrogen-bonding scheme (dashed bonds). H atoms not involved in this network have been omitted.

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