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1,4-Bis(benzimidazol-1-ylmethyl)-2,3,5,6-tetramethylbenzene methanol disolvate

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
R factor = 0.041
wR factor = 0.103
Data-to-parameter ratio = 9.9

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

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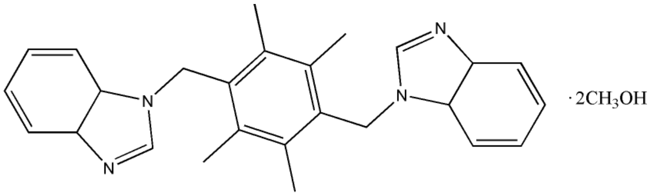
The title compound, $C_{26}H_{26}N_4 \cdot 2CH_3OH$, lies across a crystallographic inversion centre. The two benzimidazole pendant substituents adopt a *trans* conformation. O—H···N and C—H···O hydrogen bonds link the molecules into a two-dimensional network parallel to ($\bar{1}$01).

Comment

Semirigid bibenzimidazole-type bidentate ligands have been utilized by us and others to generate various coordination assemblies with varied structural topologies (Su *et al.*, 2003). It was found that this type of ligand can adopt either *trans* or *cis* conformations to give completely different structural modes. When a *trans* conformation is adopted, extended coordination polymers are formed (Su, Cai, Chen & Kang, 2001). On the other hand, discrete molecules can also be constructed with the ligands adopting a *cis* conformation (Su, Cai, Chen, Zhang & Kang, 2001). We are interested in what kind of conformation is preferred by the free ligand without coordinative interactions. We report here the crystal structure of the title compound with two solvent methanol molecules.



(I)

The title compound crystallizes in the centrosymmetric space group $P2_1/n$ and lies across a crystallographic inversion

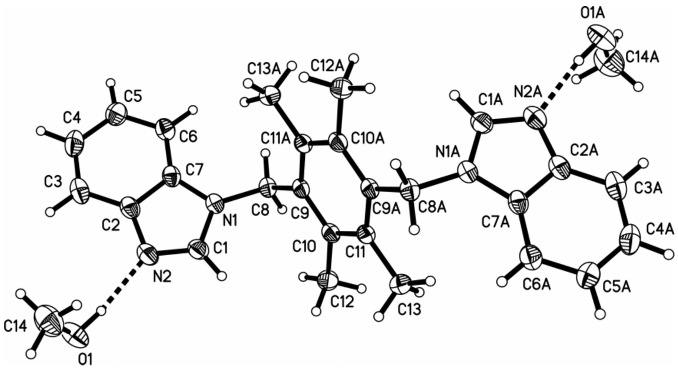


Figure 1
View of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. Atoms labelled with the suffix A are generated by the symmetry operation $(1 - x, 1 - y, 1 - z)$. Dashed lines indicate hydrogen bonds.

centre. The two benzimidazole ring systems are *trans* with respect to each other, with one pendant located above the central benzene core while the other is below, as shown in Fig. 1. The benzimidazole rings are planar within ±0.015 (1) Å, and the dihedral angle between the benzimidazole plane and the central benzene ring is 71.27 (4)°.

The two solvent methanol molecules form O—H···N hydrogen bonds with two N-atom acceptors (Table 1). In addition, symmetry-related molecules are linked to the methanol molecules *via* C—H···O hydrogen bonds, leading to the formation of a two-dimensional network parallel to ($\bar{1}$01) (Fig. 2).

Experimental

The title compound was prepared from the substitution reaction between 1*H*-benzimidazole (1.06 g, 9 mmol) and 1,4-tris(bromomethyl)-2,3,5,6-tetramethylbenzene (1.44 g, 4.5 mmol) under strong alkaline (KOH; 1.00 g, 18 mmol) conditions. Single crystals suitable for X-ray analysis were obtained by slow evaporation of a methanol solution at room temperature.

Crystal data

$C_{26}H_{26}N_4 \cdot 2CH_4O$
$M_r = 458.59$
Monoclinic, $P2_1/n$
$a = 5.2957$ (3) Å
$b = 16.2732$ (9) Å
$c = 13.9411$ (8) Å
$\beta = 93.200$ (1)°
$V = 1199.54$ (12) Å^3
$Z = 2$

$D_x = 1.27$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5358 reflections
$\theta = 2.9$–25.1°
$\mu = 0.08$ mm^{-1}
$T = 150$ (2) K
Block, colourless
0.42 × 0.20 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.967$, $T_{\max} = 0.993$
8425 measured reflections

2118 independent reflections
1903 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.048$
$\theta_{\max} = 25.1°$
$h = -6 \rightarrow 6$
$k = -19 \rightarrow 19$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.103$
$S = 1.08$
2118 reflections
214 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0504P)^2 + 0.2602P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.002$
$\Delta\rho_{\max} = 0.17$ e Å^{-3}
$\Delta\rho_{\min} = -0.16$ e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*D*···N2	0.91 (2)	1.88 (2)	2.783 (2)	170 (2)
C6—H6···O1$^{\rm i}$	0.96 (2)	2.45 (2)	3.386 (2)	168 (1)
C8—H8*A*···O1$^{\rm i}$	1.00 (2)	2.47 (2)	3.456 (2)	171 (1)

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

All H atoms were located in a difference Fourier map, except for the methyl H atoms of the solvent, which were included as riding atoms (C—H = 0.98 Å). For the refined H atoms, the O—H distance is 0.91 (2) Å and the C—H distances are in the range 0.953 (18)–1.00 (2) Å.

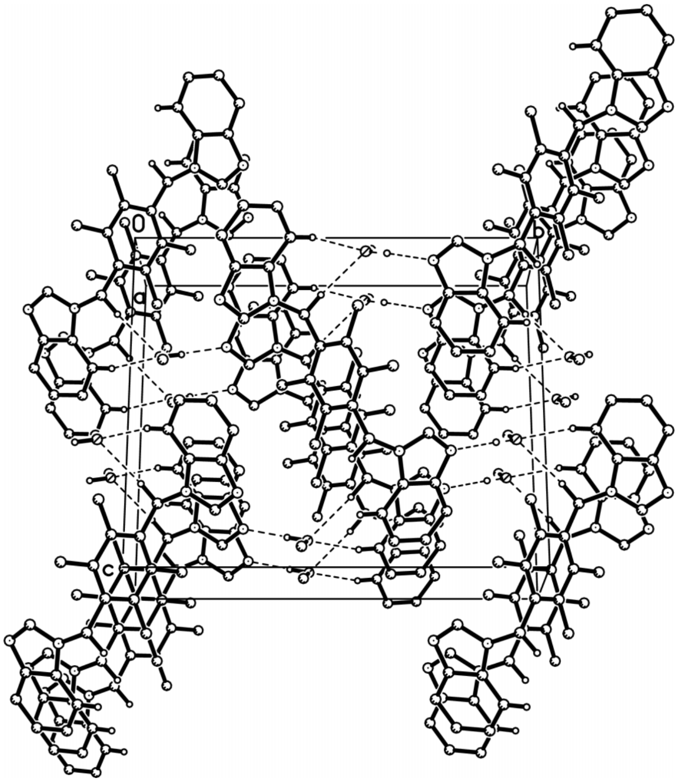


Figure 2
Crystal packing in the title compound, viewed down the *a* axis. Dashed lines indicate hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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