Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

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Electronic paper
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1*H*,1′*H*-2,2′-Bibenzimidazole

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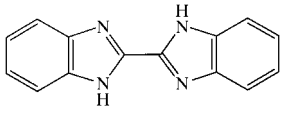
Received 29 August 2000
Accepted 18 October 2000

Data validation number: IUC0000290

In the title compound, $C_{14}H_{10}N_4$, all the atoms are close to being coplanar (r.m.s. deviation 0.0098 Å) except for the imino H atoms. The molecule forms a one-dimensional chain through intermolecular N—H···N hydrogen bonds.

Comment

The title compound, (I), is well known to act as a bridging ligand in transition metal compounds (Fieselmann *et al.*, 1978; Haga *et al.*, 1987). The asymmetric unit contains one quarter of the molecule and the other parts are twofold-rotation and mirror related. The rotation axis passes through the centre of the C1—C1′ bond, while the mirror contains this bond. The occupancy of the imino H1 atom was set at 0.5 due to the mirror-symmetry operation. The average bond distances and angles for the benzimidazole moiety are in good agreement with those of other substituted bis-benzimidazole compounds (Matthews *et al.*, 1996; Ozbey *et al.*, 1998; Bei *et al.*, 2000).



(I)

The C1—C1′ bond length of 1.435 (5) Å is close to the value for a single-bond length between trigonally linked C atoms (Cruickshank & Sparks, 1960; Bei *et al.*, 2000). The molecule forms a one-dimensional chain through N1—H1···N1(x, $-y$, $-\frac{1}{2}-z$) intermolecular hydrogen bonds.

Experimental

The title compound was prepared from 1,2-diaminobenzene and oxamide according to the method of Fieselmann *et al.* (1978). Single crystals suitable for X-ray measurement were obtained by slow evaporation at room temperature from an ethylene glycol solution.

Crystal data

$C_{14}H_{10}N_4$
$M_r = 234.26$
Orthorhombic, *Ibam*
$a = 11.331$ (3) Å
$b = 10.183$ (2) Å
$c = 9.962$ (2) Å
$V = 1149.4$ (4) Å^3
$Z = 4$
$D_x = 1.354$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 12.4$–$14.9°$
$\mu = 0.085$ mm^{-1}
$T = 296.2$ K
Prismatic, yellow
0.30 × 0.10 × 0.10 mm

Data collection

Rigaku AFC-5*R* diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.937$, $T_{max} = 0.996$
985 measured reflections
703 independent reflections
321 reflections with $I > 2\sigma(I)$
$R_{int} = 0.015$
$\theta_{max} = 27.5°$
$h = -1 \rightarrow 14$
$k = -1 \rightarrow 13$
$l = -1 \rightarrow 12$
3 standard reflections
every 150 reflections
intensity decay: 0.55%

Refinement

Refinement on F^2
$R(F) = 0.043$
$wR(F^2) = 0.127$
$S = 1.06$
703 reflections
55 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + \{0.045[\mathrm{Max}(F_o^2,0) + 2F_c^2]/3\}^2]$
$(\Delta/\sigma)_{max} = 0.004$
$\Delta\rho_{max} = 0.48$ e Å^{-3}
$\Delta\rho_{min} = -0.43$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—C1	1.339 (2)	C2—C3	1.385 (3)
N1—C2	1.394 (3)	C3—C4	1.367 (4)
C1—C1^{i}	1.436 (6)	C4—C4^{ii}	1.377 (5)
C2—C2^{ii}	1.382 (4)		
C1—N1—C2	104.7 (2)	N1—C1—C1^{i}	122.8 (1)
N1—C1—N1^{ii}	114.3 (3)	N1—C1^{ii}—C1^{i}	122.8 (1)

Symmetry codes: (i) $2-x, -y, z$; (ii) $x, y, -z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N1^{i}	0.94 (4)	1.99 (4)	2.897 (3)	160 (3)

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

All the H atoms were located from the difference Fourier map and refined isotropically. The C—H distance range is 0.92 (3)–1.01 (2) Å and the N—H distance is 0.94 (4) Å.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1990); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation and Rigaku Corporation, 1999); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *TEXSAN*; software used to prepare material for publication: *TEXSAN*.

The authors whish to acknowledge Y. Nakamura and A. Tada for their help in the preparation and recrystallization of the title compound.

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