metal-organic papers

Dibromo[*N,N*-dimethyl-*N'*-(2-pyridylmethyl-idene)propane-1,3-diamine]zinc(II)

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In the title mononuclear zinc(II) compound, [ZnBr$_2$-(C$_{11}$H$_{17}$N$_3$)], the Zn^{II} ion is five-coordinated by three N atoms of a Schiff base ligand and by two Br$^-$ anions, forming a distorted square-pyramidal geometry with a Br atom in the apical site.

Comment

Zinc complexes are very important in biology, functioning as the active site of hydrolytic enzymes, where they are in a hard-donor coordination environment of nitrogen and oxygen (Sanmartín *et al.*, 2000; Vallee & Auld, 1993). As part of an investigation of the structures of such zinc compounds, the title mononuclear zinc(II) complex, (I), was synthesized and its crystal structure is reported here.

(I)
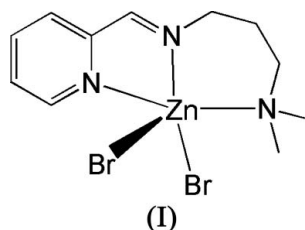
The Zn^{II} atom in (I) is five-coordinated by three N atoms of the Schiff base ligand, and by two Br atoms, forming a
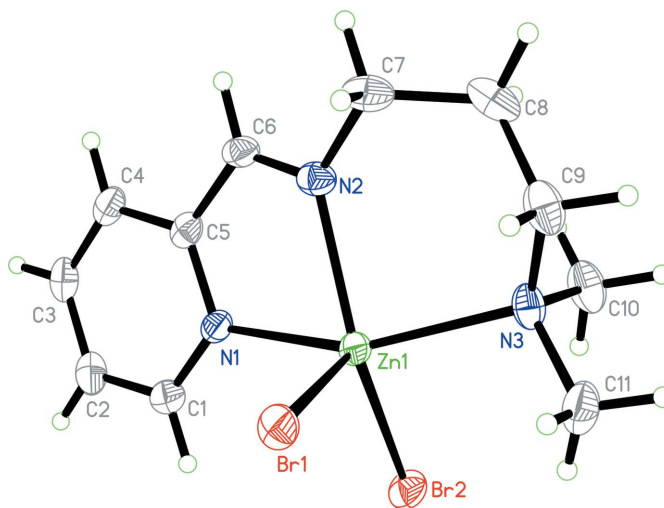
Figure 1
A view of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

distorted square-pyramidal geometry, as shown in Fig. 1. The bond lengths (Table 1) involving the Zn^{II} ion are comparable with the corresponding values observed in other zinc(II) complexes (McCleverty *et al.*, 1980; Usman *et al.*, 2003; You & Zhu, 2006). The significant distortion of the square pyramid is revealed by the bond angles between the apical Br1 atom and basal donor atoms (Table 1). As expected, the six-membered chelate ring Zn1/N2/C7–C9/N3 adopts a chair conformation. In the crystal structure, molecules are linked through weak C—H···Br interactions (Table 2).

Experimental

Compound (I) was obtained by stirring pyridine-2-carbaldehyde (1.0 mmol, 107.3 mg), *N,N*-dimethylpropane-1,3-diamine (1.0 mmol, 102.1 mg) and zinc bromide (1.0 mmol, 245.4 mg) in an EtOH solution (50 ml). The residue was recrystallized from an EtOH solution.

Crystal data

[ZnBr$_2$(C$_{11}$H$_{17}$N$_3$)]	$Z = 2$
$M_r = 416.47$	$D_x = 1.915$ Mg m^{-3}
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 7.602$ (1) Å	Cell parameters from 2250
$b = 9.150$ (2) Å	reflections
$c = 11.901$ (2) Å	$\theta = 2.5$–26.7°
$\alpha = 97.82$ (3)°	$\mu = 7.21$ mm^{-1}
$\beta = 103.30$ (3)°	$T = 298$ (2) K
$\gamma = 112.25$ (2)°	Block, yellow
$V = 722.4$ (3) Å^3	$0.20 \times 0.20 \times 0.18$ mm

Data collection

Bruker SMART CCD area-detector diffractometer	3200 independent reflections
	2502 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.041$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$\theta_{max} = 27.5°$
	$h = -9 \rightarrow 9$
$T_{min} = 0.250$, $T_{max} = 0.273$	$k = -11 \rightarrow 11$
6202 measured reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.038$	$w = 1/[\sigma^2(F_o^2) + (0.0229P)^2]$
$wR(F^2) = 0.090$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.001$
3200 reflections	$\Delta\rho_{max} = 0.68$ e Å^{-3}
156 parameters	$\Delta\rho_{min} = -0.65$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N2	2.155 (3)	Zn1—Br1	2.4163 (15)
Zn1—N1	2.227 (3)	Zn1—Br2	2.4631 (9)
Zn1—N3	2.236 (3)		
N2—Zn1—N1	74.49 (12)	N3—Zn1—Br1	101.78 (9)
N2—Zn1—N3	88.15 (13)	N2—Zn1—Br2	146.19 (9)
N1—Zn1—N3	151.26 (12)	N1—Zn1—Br2	89.05 (8)
N2—Zn1—Br1	102.52 (9)	N3—Zn1—Br2	93.38 (9)
N1—Zn1—Br1	104.21 (9)	Br1—Zn1—Br2	110.16 (4)

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

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10C···Br2	0.96	2.92	3.571 (3)	126
C11—H11A···Br2	0.96	2.85	3.536 (3)	129

H atoms were placed in idealized positions and constrained to ride on their parent atoms, C—H = 0.93–0.97 Å and with U_{iso}(H) = 1.2 or 1.5 times U_{eq}(C).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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