Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Dibromo{2-[2-(methylamino)ethyliminomethyl]phenolato}zinc(**II**)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.041
wR factor = 0.087
Data-to-parameter ratio = 21.6

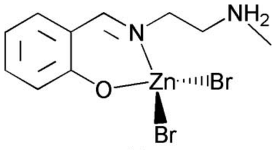
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 8 May 2006
Accepted 9 May 2006

In the title mononuclear Schiff base zinc(II) complex, [$ZnBr_2(C_{10}H_{14}N_2O)$], the Zn^{II} ion is coordinated by one O atom and one imine N atom of the Schiff base ligand and by two bromide anions, giving a four-coordinate tetrahedral geometry. The crystal structure is stabilized by intermolecular N—H···O and N—H···Br hydrogen bonds.

Comment

Zinc complexes have been of great interest in coordination chemistry related to enzymatic reactions and molecular architectures (Fabiane *et al.*, 1998; Demadis *et al.*, 2005; Hanson *et al.*, 2004; Moghimi *et al.*, 2005). As part of a further investigation of the structures of zinc complexes, the title mononuclear zinc(II) complex, (I), is reported in this paper.



(I)

In complex (I), the Zn atom is coordinated by one O atom and one imine N atom of the Schiff base ligand, and by two bromide anions, giving a four-coordinate tetrahedral geometry (Fig. 1). All the bond lengths and angles (Table 1) related to the Zn atom in the complex are comparable to the values in other zinc(II) complexes (Qiu, 2006; Odoko *et al.*, 2006; Zhang *et al.*, 2006; Peng *et al.*, 2006). As a result of the N2—H2*B*···Br1 intramolecular hydrogen bond (Table 2), the C8/

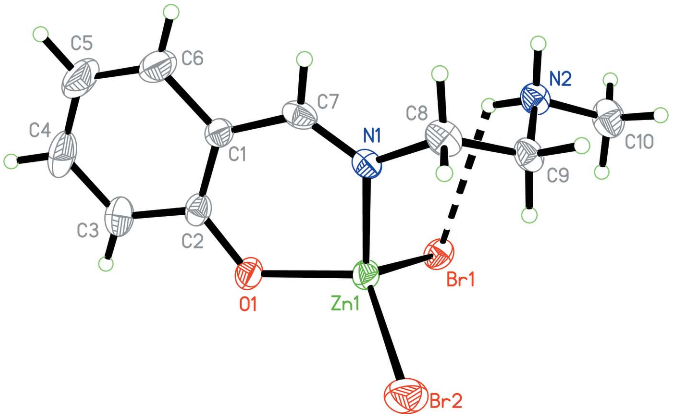


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. The intramolecular N—H···Br hydrogen bond is shown as a dashed line.

C9/N2/C10 chain is inclined towards the bromine anion Br1. The C8—C9—N2—C10 torsion angle is 3.5 (5)°.

The crystal structure is stabilized by intermolecular N—H···O and N—H···Br hydrogen bonds, forming chains running along the *b* axis (Fig. 2 and Table 2).

Experimental

Salicylaldehyde (1.0 mmol, 122.2 mg), *N*-methylethane-1,2-diamine (1.0 mmol, 75.3 mg) and zinc bromide (1.0 mmol, 145.2 mg) were dissolved in ethanol (60 ml). The mixture was stirred for about 1 h to give a clear colourless solution. After keeping the solution in air for 17 d, colourless block-like crystals were formed.

Crystal data

$[ZnBr_2(C_{10}H_{14}N_2O)]$
$M_r = 403.42$
Monoclinic, $P2_1/n$
$a = 10.599$ (2) Å
$b = 7.426$ (1) Å
$c = 17.624$ (3) Å
$\beta = 90.990$ (2)°
$V = 1387.0$ (4) Å^3
$Z = 4$
$D_x = 1.932$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 7.52$ mm^{-1}
$T = 298$ (2) K
Block, colourless
0.18 × 0.16 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.345$, $T_{max} = 0.399$ (expected range = 0.280–0.324)
11411 measured reflections
3155 independent reflections
2089 reflections with $I > 2\sigma(I)$
$R_{int} = 0.055$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.087$
$S = 1.00$
3155 reflections
146 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0298P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.73$ e Å^{-3}
$\Delta\rho_{min} = -0.56$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.938 (3)	Zn1—Br2	2.3334 (9)
Zn1—N1	2.005 (3)	Zn1—Br1	2.3959 (8)
O1—Zn1—N1	96.78 (13)	O1—Zn1—Br1	108.76 (9)
O1—Zn1—Br2	112.53 (10)	N1—Zn1—Br1	109.04 (9)
N1—Zn1—Br2	110.72 (10)	Br2—Zn1—Br1	117.10 (3)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*B*···Br1	0.90	2.96	3.562 (3)	126
N2—H2*B*···Br1^{i}	0.90	2.69	3.465 (3)	145
N2—H2*A*···O1^{ii}	0.90	1.92	2.808 (4)	170

Symmetry codes: (i) $-x, -y+2, -z$; (ii) $x, y+1, z$.

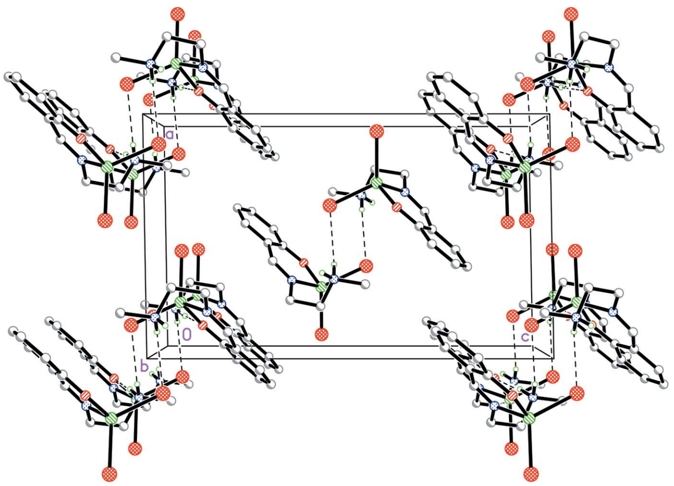


Figure 2
The crystal packing of (I), viewed along the *b* axis. Intermolecular hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

All H atoms were placed in idealized positions and constrained to ride on their parent atoms. Constrained distances: N—H = 0.90 Å, C—H = 0.93 Å for aromatic CH groups, 0.96 Å for methylene CH_2, and 0.97 Å for methyl CH_3. Isotropic displacement parameters were fixed at $U_{iso}(H) = 1.2U_{iso}(C,N)$ for the amine N atom and methylene CH_2 groups and $1.5U_{iso}(C)$ for the methyl group.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); 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*.

The authors acknowledge Henan University of Science and Technology for a research grant.

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