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Dibromo{2-[3-(methylamino)propylimino-methyl]phenolato}zinc(II)

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The title compound, $[ZnBr_2(C_{11}H_{16}N_2O)]$, is a mononuclear Schiff base zinc(II) complex. The Zn^{II} atom is four-coordinated by one phenolate O and one imine N atom of the Schiff base ligand, and by two bromide anions, forming a tetrahedral coordination. In the crystal structure, molecules are linked through intermolecular N—H···O and N—H···Br hydrogen bonds, forming sheets parallel to the *ab* plane.

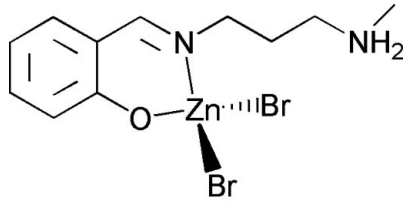
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.008 Å
R factor = 0.046
wR factor = 0.119
Data-to-parameter ratio = 21.9

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

Comment

Zinc(II) complexes are very important in biological chemistry (Weston, 2005; Henkel & Krebs, 2004). They function as the active site of hydrolytic enzymes, such as carboxypeptidase and carbonic anhydrase (Bertini *et al.*, 1994; Lipscomb & Sträter, 1996). The crystal structure of a new zinc(II) complex derived from the Schiff base 2-[3-(methylamino)propyliminomethyl]phenol is reported here.



(I)

The title compound, (I), is a mononuclear Schiff base zinc(II) complex (Fig. 1). The Zn^{II} atom is four-coordinated by one phenolate O and one imine N atom of the Schiff base ligand, and by two bromide anions, forming a tetrahedral coordination. The Zn—O and Zn—N bond lengths (Table 1) are comparable with the corresponding values observed in other Schiff base zinc(II) complexes (Tatar *et al.*, 1999; You & Zhu, 2006; Hou, 2005). As expected, the N1–C8–C9–C10–N2–C11 chain adopts a *trans* conformation to minimize steric effects.

In the crystal structure, the molecules are linked through intermolecular N—H···O and N—H···Br hydrogen bonds (Table 2), forming sheets parallel to the *ab* plane (Fig. 2).

Experimental

A mixture of salicylaldehyde (1.0 mmol, 122.1 mg), *N*-methyl-1,3-diaminopropane (1.0 mmol, 88.3 mg) and $ZnBr_2$ (1.0 mmol, 225.4 mg) was dissolved in ethanol (100 ml). The mixture was stirred for 1 h at room temperature to give a clear colourless solution. After allowing the solution to stand still in air for 12 d, colourless block-shaped crystals had formed.

Crystal data

$[ZnBr_2(C_{11}H_{16}N_2O)]$
M_r = 417.45
Orthorhombic, *Pbca*
a = 11.757 (2) Å
b = 14.363 (2) Å
c = 17.535 (2) Å
V = 2961.1 (7) Å^3
Z = 8
D_x = 1.873 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2896 reflections
θ = 2.3–24.6°
μ = 7.04 mm^{-1}
T = 298 (2) K
Block, colourless
0.22 × 0.20 × 0.19 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.231, T_{max} = 0.262
23813 measured reflections
3401 independent reflections
2064 reflections with $I > 2\sigma(I)$
R_{int} = 0.093
θ_{max} = 27.5°
$h = -15 \rightarrow 15$
$k = -18 \rightarrow 18$
$l = -22 \rightarrow 22$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.119
S = 1.01
3401 reflections
155 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0455P)^2 + 2.7431P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.94 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.946 (3)	Zn1—Br2	2.3492 (10)
Zn1—N1	1.996 (4)	Zn1—Br1	2.3957 (9)
O1—Zn1—N1	96.15 (16)	O1—Zn1—Br1	111.44 (12)
O1—Zn1—Br2	109.04 (12)	N1—Zn1—Br1	105.66 (14)
N1—Zn1—Br2	120.13 (14)	Br2—Zn1—Br1	113.18 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1^{i}	0.90	1.84	2.733 (5)	173
N2—H2B···Br1^{ii}	0.90	2.49	3.381 (4)	170

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

H atoms were placed in calculated positions and constrained to ride on their parent atoms, with N—H = 0.90 Å, C—H = 0.93–0.97 Å and U_{iso}(H) = 1.2 or 1.5U_{eq}(C,N).

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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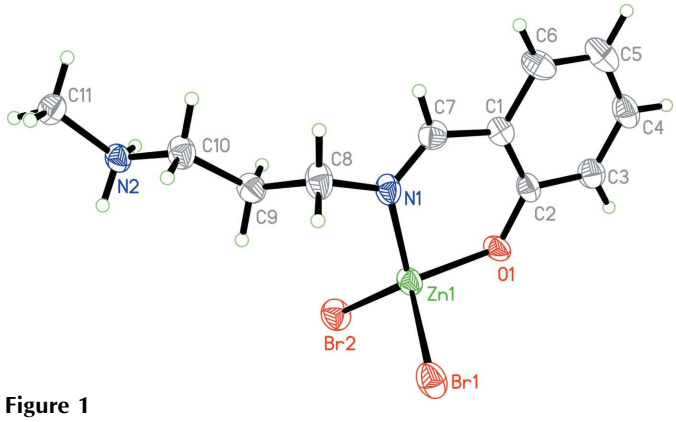

Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids.

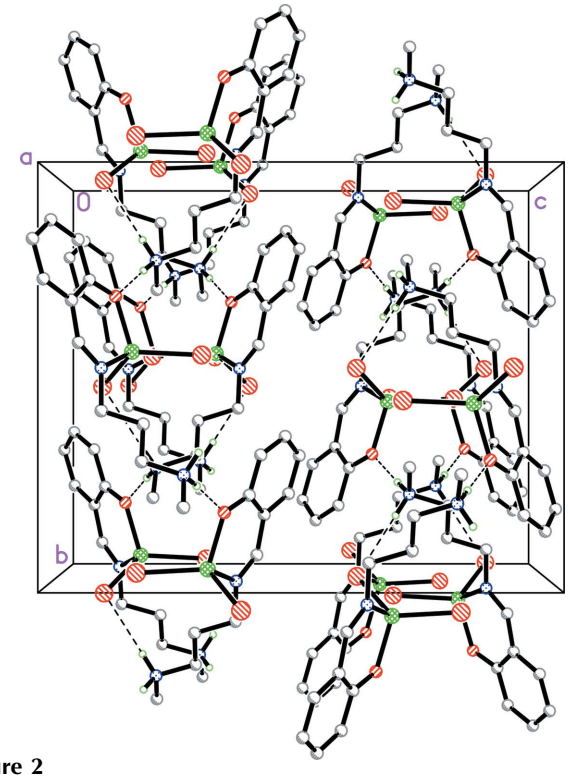

Figure 2
The crystal packing of (I). Intermolecular N—H···O and N—H···Br hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

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