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# Dibromido{4-chloro-2-[3-(dimethylamino)-propyliminomethyl]phenolato}zinc(II)

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**Key indicators**

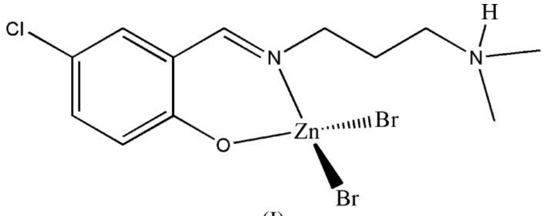
Single-crystal X-ray study
$T$ = 298 K
Mean $\sigma$(C–C) = 0.011 Å
$R$ factor = 0.060
$wR$ factor = 0.179
Data-to-parameter ratio = 19.6

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

The title compound, [$ZnBr_2(C_{12}H_{17}ClN_2O)$], is a mononuclear Schiff base zinc(II) complex. The Zn atom in the compound is four-coordinated by one imine N and one phenolate O atom of the Schiff base ligand and by two terminal Br anions, forming a tetrahedral geometry. In the crystal structure, molecules are linked through intermolecular N—H···O hydrogen bonds, forming chains running along the $c$ axis.

## Comment

The condensation reaction of aromatic carbaldehydes with primary amines has been shown to offer an easy and inexpensive way of forming a variety of polydentate Schiff base ligands. Zinc(II) complexes derived from Schiff base ligands have been studied extensively due to their interesting structures and wide applications (Lacroix *et al.*, 1996; Chisholm *et al.*, 2001; Jian *et al.*, 2004; Tatar *et al.*, 2002; Bhosekar *et al.*, 2006). As part of a further investigation of the structures of such Schiff base zinc(II) complexes (Wei *et al.*, 2007), the title mononuclear zinc(II) complex, (I), is reported here.



(I)

The tetrahedral coordination of the $Zn^{II}$ atom in (I) is formed by one imine N and one phenolate O atom of the Schiff base ligand and by two terminal Br anions (Fig. 1). The coordination bond distances (Table 1) are typical and comparable with the values in other similar zinc(II) complexes (Peng & Hou, 2006; Peng *et al.*, 2006; Ma & Gu *et al.*, 2006; Ma & Lv *et al.*, 2006). The O1—Zn1—N1 and Br1—Zn1—Br2 bond angles deviate most from ideal tetrahedral geometry, with values of 93.8 (2) and 115.39 (5)°, respectively. The other angles in the coordination environment are in the range 108.23 (17)–114.92 (19)° (Table 1).

In the crystal structure of (I), molecules are linked through intermolecular N—H···O hydrogen bonds (Table 2), forming chains running along the $c$ axis.

## Experimental

Compound (I) was obtained by stirring 5-chlorosalicylaldehyde (0.1 mmol, 15.7 mg), *N*,*N*-dimethyl-1,3-diaminopropane (0.1 mmol, 10.2 mg), and zinc(II) bromide (0.1 mmol, 22.5 mg) in methanol

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(20 ml) for 30 min at room temperature. The reaction mixture was then filtered. Colourless block-shaped single crystals suitable for X-ray diffraction formed from the filtrate after three days.

### *Crystal data*

$[ZnBr_2(C_{12}H_{17}ClN_2O)]$
$M_r = 465.92$
Monoclinic, $P2_1/n$
$a = 7.103$ (1) Å
$b = 14.851$ (2) Å
$c = 16.058$ (2) Å
$\beta = 91.886$ (2)°
$V = 1693.0$ (4) $Å^3$
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 6.32$ $mm^{-1}$
$T = 298$ (2) K
0.19 × 0.11 × 0.11 mm

### *Data collection*

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.380$, $T_{max} = 0.543$ (expected range = 0.349–0.499)
12802 measured reflections
3481 independent reflections
2178 reflections with $I > 2\sigma(I)$
$R_{int} = 0.065$

### *Refinement*

$R[F^2 > 2\sigma(F^2)] = 0.060$
$wR(F^2) = 0.179$
$S = 1.02$
3481 reflections
178 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.66$ e $Å^{-3}$
$\Delta\rho_{min} = -1.21$ e $Å^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Zn1—O1 | 1.952 (5) | Zn1—Br1 | 2.3354 (14) |
| Zn1—N1 | 2.014 (6) | Zn1—Br2 | 2.3830 (15) |
| | | | |
| O1—Zn1—N1 | 93.8 (2) | O1—Zn1—Br2 | 114.92 (19) |
| O1—Zn1—Br1 | 110.53 (17) | N1—Zn1—Br2 | 108.23 (17) |
| N1—Zn1—Br1 | 111.95 (18) | Br1—Zn1—Br2 | 115.39 (5) |

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2···O1$^{i}$ | 0.89 (6) | 1.97 (6) | 2.859 (9) | 174 (7) |

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

Atom H2 was located in a difference Fourier map and refined isotropically, with the N—H distance restrained to 0.90 (1) Å. Other H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding, with $U_{iso}(H)$ values set at 1.2 or $1.5U_{eq}(C)$. The deepest residual electron density hole is located 0.63 Å from atom Br2.

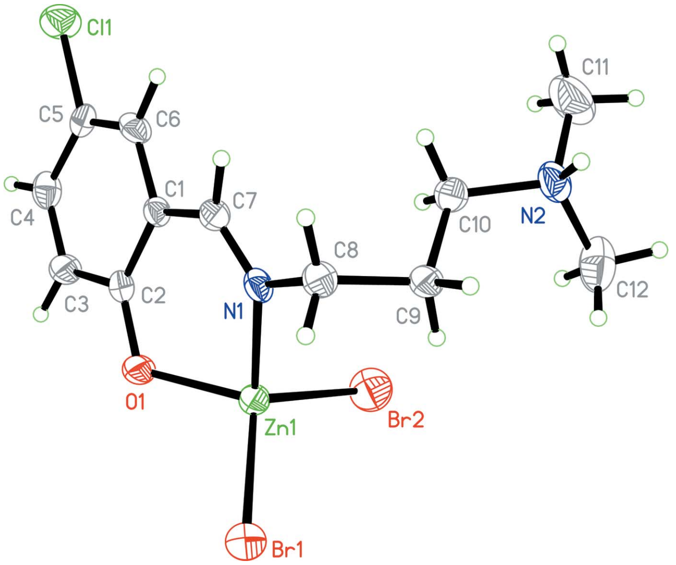

**Figure 1**
The molecular structure of (I), shown with 30% probability displacement ellipsoids.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXTL*.

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