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# Dibromo{4-bromo-2-[2-(isopropylamino)-ethyliminomethyl]phenolato}zinc(II)

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**Key indicators**

Single-crystal X-ray study
*T* = 298 K
Mean σ(C–C) = 0.013 Å
*R* factor = 0.072
*wR* factor = 0.215
Data-to-parameter ratio = 19.9

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



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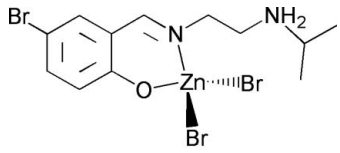
In the title mononuclear Schiff base zinc(II) complex, $[ZnBr_2(C_{12}H_{17}BrN_2O)]$, the $Zn^{II}$ ion is four-coordinated by one O atom and one imine N atom of a Schiff base ligand, and by two Br atoms, giving a tetrahedral geometry. The crystal structure is stabilized by intermolecular C—H···O hydrogen 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). In a further investigate of the structures of zinc complexes, the title mononuclear zinc(II) complex, (I), is reported here.




(I)

In complex (I), the Zn atom is four-coordinated by one O atom and one imine N atom of a Schiff base ligand, and by two Br atoms, giving a tetrahedral geometry (Fig. 1). All of the bond lengths and angles (Table 1) involving the Zn atom are comparable to the values in other zinc(II) complexes (Qiu, 2006; Odoko *et al.*, 2006; Zhang, 2006; Peng *et al.*, 2006). The C8—C9—N2—C10, C9—N2—C10—C11 and C9—N2—C10—C12 torsion angles are 17.0 (6), 60.1 (7) and 1.4 (7)°, respectively.

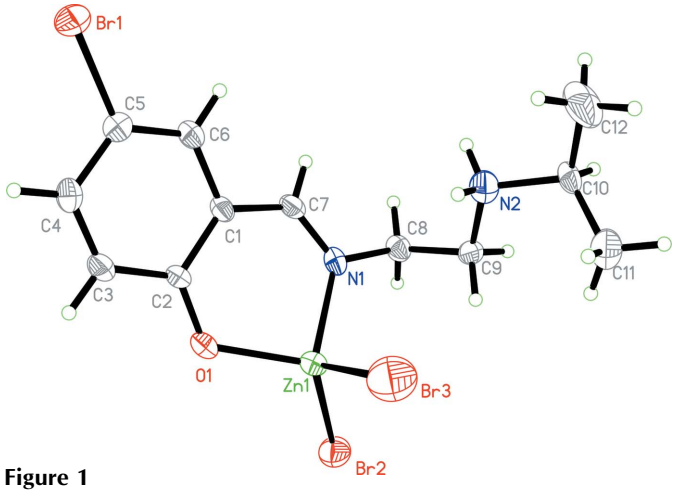



**Figure 1**
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

In the crystal structure, the molecules are stabilized by intermolecular C—H···O hydrogen bonds, forming layers parallel to the *bc* plane (Fig. 2 and Table 2).

## Experimental

5-Bromosalicylaldehyde (1.0 mmol, 201.3 mg), *N*-isopropylethane-1,2-diamine (1.0 mmol, 102.2 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 leaving the solution to stand in air for 13 d, colourless block-like crystals were formed.

*Crystal data*

$[ZnBr_2(C_{12}H_{17}BrN_2O)]$
$M_r$ = 510.38
Monoclinic, $P2_1/n$
$a$ = 7.044 (1) Å
$b$ = 15.048 (3) Å
$c$ = 16.179 (3) Å
$\beta$ = 92.007 (3)°
$V$ = 1713.9 (5) Å$^3$
$Z$ = 4
$D_x$ = 1.978 Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu$ = 8.42 mm$^{-1}$
$T$ = 298 (2) K
Block, colourless
0.12 × 0.10 × 0.09 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.431, $T_{max}$ = 0.518
(expected range = 0.390–0.469)
13301 measured reflections
3471 independent reflections
2078 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.075
$\theta_{max}$ = 26.5°

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.072
$wR(F^2)$ = 0.215
$S$ = 1.05
3471 reflections
174 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1122P)^2 + 0.0647P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.96 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.86 e Å$^{-3}$

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

| | | | |
|---|---|---|---|
| Zn1—O1 | 1.944 (7) | Zn1—Br2 | 2.3382 (16) |
| Zn1—N1 | 2.007 (8) | Zn1—Br3 | 2.402 (2) |
| O1—Zn1—N1 | 94.3 (3) | O1—Zn1—Br3 | 116.7 (2) |
| O1—Zn1—Br2 | 110.6 (2) | N1—Zn1—Br3 | 105.8 (2) |
| N1—Zn1—Br2 | 112.4 (2) | Br2—Zn1—Br3 | 115.01 (7) |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C10—H10···O1$^{i}$ | 0.98 | 1.91 | 2.882 (11) | 170 |

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

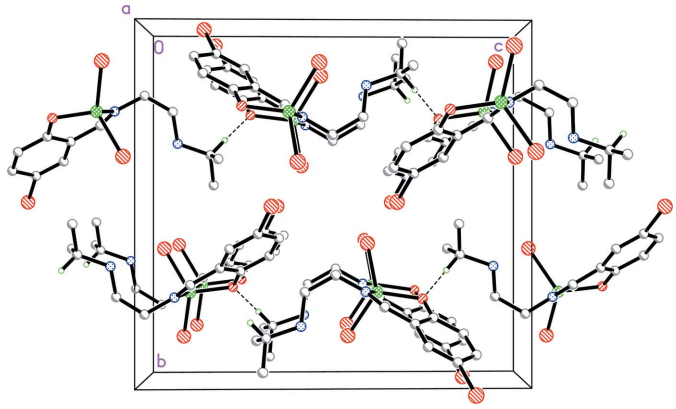



**Figure 2**
The packing of (I), viewed along the *a* axis. Intermolecular hydrogen bonds are shown as dashed lines.

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, C—H = 0.97 Å for methylene $CH_2$ groups and C—H = 0.96 Å for methyl $CH_3$ groups. Isotropic displacement parameters were fixed at $U_{iso}$(H) = 1.2$U_{iso}$(C,N) for amine and methylene $CH_2$ groups and at 1.5$U_{iso}$(C) for methyl $CH_3$ groups. The maximum residual density was observed 1.15 Å from Br3 and the minimum residual density was observed 0.56 Å from atom Br3.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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, 1998); software used to prepare material for publication: *SHELXTL*.

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## References

Bruker (1998). *SMART* (Version 5.628), *SAINT* (Version 6.02) and *SHELXTL* (Version 5.1). Bruker AXS Inc., Madison, Wisconsin, USA.
Demadis, K. D., Mantzaridis, C., Raptis, R. G. & Mezei, G. (2005). *Inorg. Chem.* **44**, 4469–4471.
Fabiane, S. M., Sohi, M. K., Wan, T., Payne, D. J., Bateson, J. H., Mitchell, T. & Sutton, B. J. (1998). *Biochemistry*, **37**, 12404–12411.
Hanson, K., Calin, N., Bugaris, D., Scancella, M. & Sevov, S. C. (2004). *J. Am. Chem. Soc.* **126**, 10502–10503.
Moghimi, A., Sheshmani, S., Shokrollahi, A., Shamsipur, M., Kickelbick, G. & Aghabozorg, H. (2005). *Z. Anorg. Allg. Chem.* **631**, 160–169.
Odoko, M., Tsuchida, N. & Okabe, N. (2006). *Acta Cryst.* E**62**, m710–m711.
Peng, S.-J., Zhou, C.-S. & Yang, T. (2006). *Acta Cryst.* E**62**, m1147–m1149.
Qiu, X.-Y. (2006). *Acta Cryst.* E**62**, m717–m718.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Zhang, Y.-L. (2006). *Acta Cryst.* E**62**, m902–m903.