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Dichlorido{2,4-dibromo-6-[2-(ethylammonio)-ethyliminomethyl]phenolato}zinc(II)

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In the title mononuclear zinc(II) complex, $[ZnCl_2(C_{11}H_{14}Br_2N_2O)]$, the Zn atom is four-coordinated by the imine N and the O atoms of the Schiff base ligand, and by two terminal chloride anions, forming a tetrahedral geometry. In the crystal structure, molecules are linked through intermolecular N—H···Cl hydrogen bonds, forming a two-dimensional network.

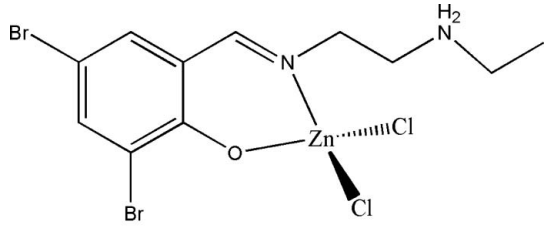
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.008 Å
R factor = 0.043
wR factor = 0.108
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

Recently, we have reported the structure of a Schiff base–nickel(II) complex (Hu *et al.*, 2005). Zinc complexes derived from Schiff base ligands possess interesting structures with wide applications (Lacroix *et al.*, 1996; Bhosekar *et al.*, 2006), and the crystal structure of the title compound, (I), is reported here.



(I)

The Zn atom in (I) is in a tetrahedral coordination, and is coordinated by the imine N and the O atoms of the Schiff base ligand and by two terminal Cl anions (Fig. 1). The bond distances (Table 1) are typical and comparable to the values in other similar zinc(II) complexes (Ma, Gu *et al.*, 2006; Ma, Lv *et*

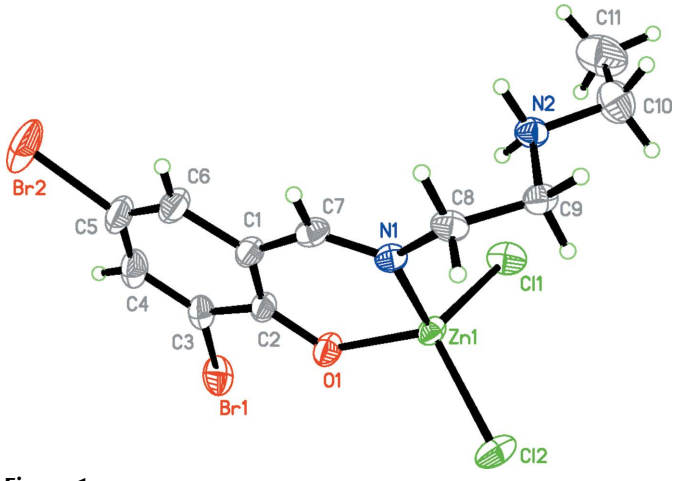


Figure 1
The molecular structure of (I), shown with 30% probability displacement ellipsoids.

al., 2006; You *et al.*, 2006). The O1—Zn1—N1 and N1—Zn1—Cl2 angles deviate most from an ideal tetrahedral geometry with values of 96.91 (14) and 116.12 (10)°, respectively. The other angles in the coordination environment are in the range 110.52 (11)–111.13 (11)° (Table 1).

In the crystal structure, molecules of (I) are linked through intermolecular N—H···Cl hydrogen bonds (Table 2), forming a two-dimensional network (Fig. 2).

Experimental

3,5-Dibromosalicylaldehyde (0.1 mmol, 28.0 mg), *N*-ethyl-1,2-diaminoethane (0.1 mmol, 8.8 mg) and zinc(II) chloride (0.1 mmol, 13.5 mg) were mixed in methanol (20 ml). The mixture was stirred for 30 min at room temperature and then fitered. Colourless block-shaped single crystals suitable for X-ray diffraction were formed from the filtrate after a week. Analysis found: C 27.36, H 2.98, N 5.60%; calculated for $C_{11}H_{14}Br_2Cl_2N_2OZn$: C 27.17, H 2.90, N 5.76%.

Crystal data

$[ZnCl_2(C_{11}H_{14}Br_2N_2O)]$
M_r = 486.33
Monoclinic, $P2_1/c$
a = 11.300 (1) Å
b = 13.654 (2) Å
c = 10.729 (1) Å
β = 94.024 (2)°
V = 1651.3 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 6.64 mm^{-1}
T = 298 (2) K
0.18 × 0.17 × 0.15 mm

Data collection

Bruker SMART APEX CCD area diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.381, T_{max} = 0.436
(expected range = 0.323–0.369)
9746 measured reflections
3788 independent reflections
2531 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.108
S = 1.02
3788 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.93 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.921 (3)	Zn1—Cl2	2.2147 (12)
Zn1—N1	2.011 (4)	Zn1—Cl1	2.2481 (14)
O1—Zn1—N1	96.91 (14)	O1—Zn1—Cl1	110.71 (11)
O1—Zn1—Cl2	111.13 (11)	N1—Zn1—Cl1	110.52 (11)
N1—Zn1—Cl2	116.12 (10)	Cl2—Zn1—Cl1	110.72 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···Cl2^{i}	0.90	2.34	3.221 (4)	167
N2—H2B···Cl1	0.90	2.42	3.181 (4)	143
N2—H2B···Cl2^{ii}	0.90	2.84	3.320 (4)	115

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

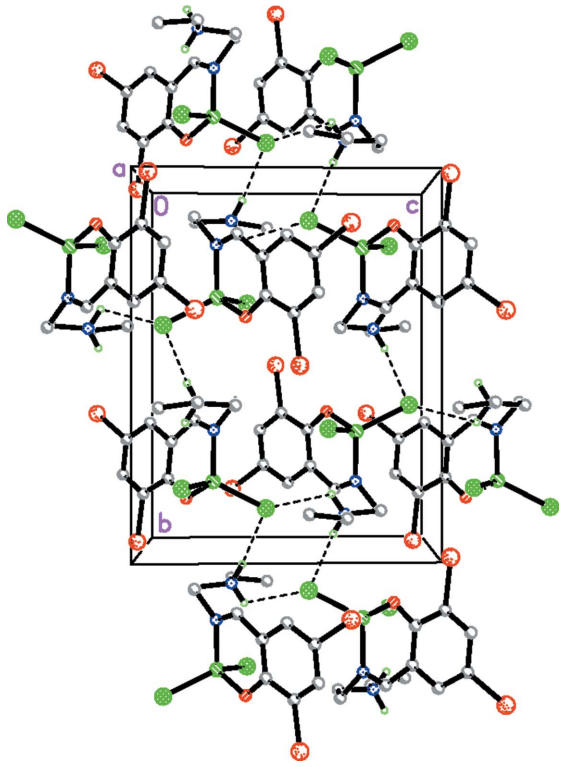


Figure 2
The molecular packing of (I), viewed along the *a* axis. Intermolecular hydrogen bonds are shown as dashed lines.

All H atoms were positioned geometrically (C—H = 0.93–0.97 Å and N—H = 0.90 Å) and refined as riding, with U_{iso}(H) values set at 1.2 or 1.5U_{eq}(C,N). The highest residual electron density peak is located 1.03 Å from Br2.

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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References

Bhosekar, G., Jess, I. & Näther, C. (2006). *Acta Cryst.* E**62**, m2073–m2074.
Bruker (1998). *SMART* (Version 5.628) and *SAINT* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
Hu, Z.-Q., Li, W.-H., Ding, Y. & Wu, Y. (2005). *Acta Cryst.* E**61**, m2526–m2527.
Lacroix, P. G., Di Bella, S. & Ledoux, I. (1996). *Chem. Mater.* **8**, 541–545.
Ma, J.-Y., Gu, S.-H., Guo, J.-W., Lv, B.-L. & Yin, W.-P. (2006). *Acta Cryst.* E**62**, m1437–m1438.
Ma, J.-Y., Lv, B.-L., Gu, S.-H., Guo, J.-W. & Yin, W.-P. (2006). *Acta Cryst.* E**62**, m1322–m1323.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
You, Z.-L., Wang, J. & Han, X. (2006). *Acta Cryst.* E**62**, m714–m716.