Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Dibromido{2,4-dichloro-6-[3-(dimethylammonio)propyliminomethyl]phenolato}zinc(II)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.008 Å
R factor = 0.050
wR factor = 0.111
Data-to-parameter ratio = 21.6

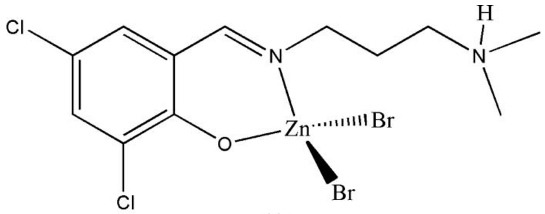
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 3 March 2007
Accepted 24 March 2007

The title compound, $[ZnBr_2(C_{12}H_{16}Cl_2N_2O)]$, is a mononuclear Zn^{II} complex. The Zn^{II} ion is four-coordinated in a tetrahedral geometry by one Schiff base ligand and by two Br atoms. In the crystal structure, molecules are linked through N—H···Br, C—H···Br and C—H···O intermolecular hydrogen bonds, forming layers parallel to the *ab* plane.

Comment

Metal complexes with Schiff bases have been of interest for a long time (Jain & Chaturvedi, 1977; Chang *et al.*, 1998; Yamada, 1999). These complexes play an important role in coordination chemistry related to catalysis and enzymatic reactions, magnetism and molecular architectures (Costamagna *et al.*, 1992; Bhatia *et al.*, 1981). The Zn^{II} ion is very effective in urease inhibition (Park & Hausinger, 1996; Ciurli *et al.*, 1999). Recently, we have reported a Schiff base–Zn^{II} complex (Li & You, 2007). As an extension of the work on these complexes, the title complex, (I), is reported here.



(I)

Compound (I) is a mononuclear Zn^{II} complex (Fig. 1). The Zn^{II} ion is four-coordinated by one O and one imine N atom of the Schiff base ligand and by two Br atoms, forming a distorted tetrahedral coordination geometry. The Schiff base ligand is in zwitterionic form, with the hydroxy group deprotonated and the dimethylamine group protonated. The bond lengths and angles around Zn (Table 1) are comparable to those observed in other Schiff base–Zn^{II} complexes (e.g. Ma, Lv *et al.*, 2006; Ma, Gu *et al.*, 2006) and those cited above.

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

Experimental

N,*N*-Dimethylpropane-1,3-diamine and 3,5-dichlorosalicylaldehyde were available commercially and were used without further purification. *N*,*N*-Dimethylpropane-1,3-diamine (0.1 mmol, 10.2 mg) and 3,5-dichlorosalicylaldehyde (0.1 mmol, 19.1 mg) were dissolved in a methanol solution (10 ml). The mixture was stirred at room temperature for 30 min, giving a clear yellow solution. To this solution was added a methanol solution (5 ml) of $ZnBr_2$ (0.1 mmol, 22.5 mg) with stirring. The resulting mixture was stirred for another 30 min at room temperature, giving a clear colourless solution. After keeping the solution in air for 3 days, colourless block-shaped crystals formed at the bottom of the vessel. Analysis found: C 28.62, H 3.27, N 5.72%; calculated for $C_{12}H_{16}Br_2Cl_2N_2OZn$: C 28.80, H 3.22, N 5.60%.

Crystal data

$[ZnBr_2(C_{12}H_{16}Cl_2N_2O)]$
$M_r = 500.36$
Orthorhombic, *Pbca*
$a = 8.235$ (1) Å
$b = 14.573$ (2) Å
$c = 29.099$ (3) Å
$V = 3492.1$ (7) Å^3
$Z = 8$
Mo $K\alpha$ radiation
$\mu = 6.29$ mm^{-1}
$T = 298$ (2) K
$0.26 \times 0.22 \times 0.21$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.222$, $T_{max} = 0.268$
27938 measured reflections
4017 independent reflections
2737 reflections with $I > 2\sigma(I)$
$R_{int} = 0.069$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.111$
$S = 1.04$
4017 reflections
186 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 1.64$ e Å^{-3}
$\Delta\rho_{min} = -1.61$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.943 (4)	Zn1—Br1	2.3668 (10)
Zn1—N1	2.016 (4)	Zn1—Br2	2.3694 (9)
O1—Zn1—N1	94.94 (17)	O1—Zn1—Br2	110.28 (12)
O1—Zn1—Br1	113.62 (14)	N1—Zn1—Br2	112.53 (13)
N1—Zn1—Br1	111.64 (13)	Br1—Zn1—Br2	112.64 (4)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···Br2^{i}	0.91 (5)	2.57 (4)	3.391 (5)	151 (6)
C10—H10*A*···O1^{i}	0.97	2.36	3.300 (5)	163
C11—H11*A*···Br1^{ii}	0.96	2.84	3.726 (5)	154

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

Atom H2 was located in a difference map and refined isotropically, with an N—H distance restraint of 0.90 (1) Å. Other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å and with $U_{iso}(H) = 1.2$ or $1.5U_{eq}(C)$. The largest residual electron density peak lies 0.93 Å from Br1, while the deepest hole lies 0.81Å from Br1.

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*.

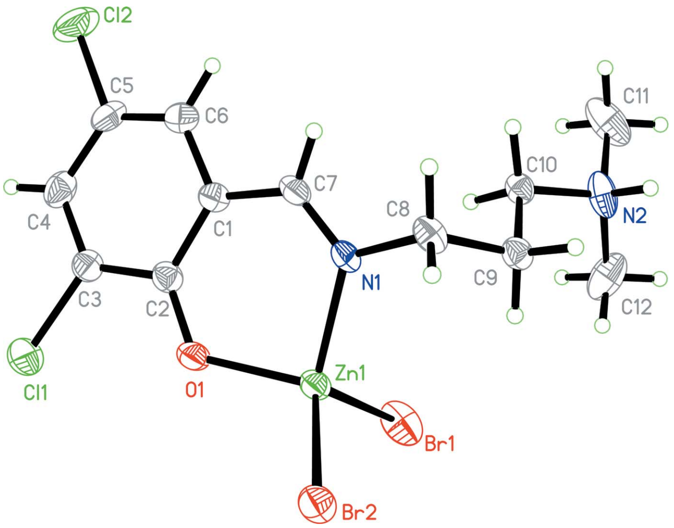


Figure 1
View of the molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

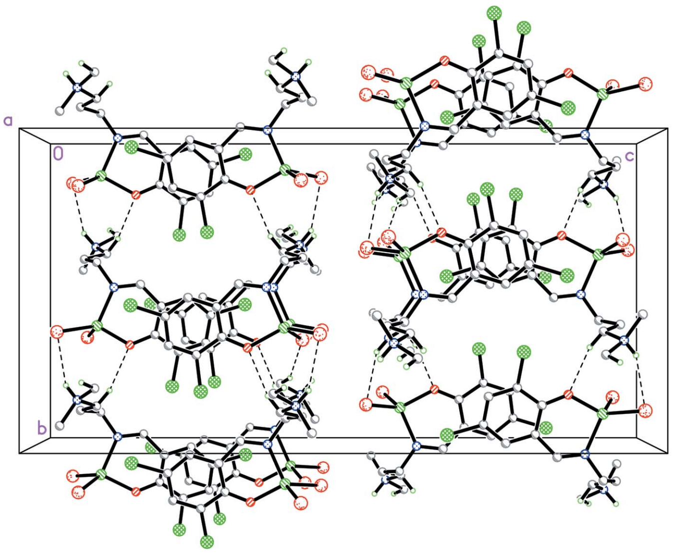


Figure 2
The crystal packing of (I), viewed along the *a* axis. Intermolecular hydrogen bonds are shown as dashed lines.

The project is sponsored by the Scientific Research Foundation for the Returned Overseas Chinese Scholars, State Education Ministry (BZYO 7002).

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