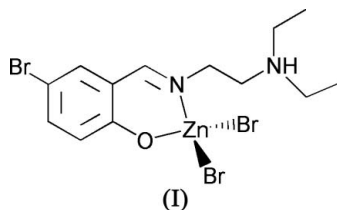


**Zhong-Lu You,* Jia Wang and
Xiao Han**Department of Chemistry and Chemical
Engineering, Liaoning Normal University,
Dalian 116029, People's Republic of ChinaCorrespondence e-mail:
youzhonglu@yahoo.com.cn**Key indicators**Single-crystal X-ray study
 $T = 298\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.010\text{ \AA}$
 R factor = 0.053
 wR factor = 0.139
Data-to-parameter ratio = 21.5For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**Dibromo{4-bromo-2-[2-(diethylaminoethyl)-
iminomethyl]phenolato}zinc(II)**

The title compound, $[\text{ZnBr}_2(\text{C}_{13}\text{H}_{19}\text{BrN}_2\text{O})]$, is a mononuclear zinc(II) complex. The Zn^{II} atom is four-coordinated in a tetrahedral configuration by one imine N and one phenolate O atoms of the Schiff base ligand, and by two terminal Br atoms. In the crystal structure, the molecules are linked through weak $\text{Br}\cdots\text{Br}$ interactions, forming chains running along $[20\bar{1}]$.

Received 1 March 2006
Accepted 2 March 2006**Comment**

Transition metal complexes containing Schiff bases have been of great interest for many years (Chaturvedi, 1977; Archer & Wang, 1990; Chang *et al.*, 1998; Yamada, 1999). These complexes play an important role in the development of coordination chemistry related to catalysis and enzymatic reactions, magnetism and molecular architectures (Costa-magna *et al.*, 1992; Bhatia *et al.*, 1981). The zinc ion is very effective in urease inhibition (Park & Hausinger, 1996; Ciurli *et al.*, 1999). The crystal structures of a few Schiff base zinc(II) complexes have already been reported from this laboratory (You, 2005*a,b,c*). As an extension of the work on these complexes, the title zinc(II) complex, (I), is reported here.



Compound (I) is a mononuclear zinc(II) complex (Fig. 1). The Zn^{II} atom is four-coordinated by one imine N and one phenolate O atoms from a Schiff base ligand, and by two terminal Br atoms, forming a tetrahedral coordination geometry. The Zn–N and Zn–O bond lengths and angles (Table 1) are comparable to the values observed in the Schiff base zinc(II) complexes cited above. There is an intramolecular N–H \cdots Br hydrogen bond (Table 2).

In the crystal structure, molecules are linked through weak $\text{Br}\cdots\text{Br}$ interactions [$\text{Br}1\cdots\text{Br}2^i = 3.672(4)\text{ \AA}$; symmetry code: (i) $1 + x, \frac{1}{2} - y, -\frac{1}{2} + z$], forming chains running along $[20\bar{1}]$ (Fig. 2).

Experimental

N,N-Diethylethane-1,2-diamine and 5-chlorosalicylaldehyde were available commercially and were used without further purification. *N,N*-Diethylethane-1,2-diamine (0.1 mmol, 11.6 mg) and 5-chlorosalicylaldehyde (0.1 mmol, 15.7 mg) were dissolved in MeOH (10 ml).

The mixture was stirred at room temperature for 30 min to give a clear yellow solution. To this solution was added an MeOH 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. After keeping the filtrate in air for 12 d, colourless block-shaped crystals were formed at the bottom of the vessel. Analysis found: C 29.77, H 3.65, N 5.34%; calculated for $\text{C}_{13}\text{H}_{19}\text{Br}_3\text{N}_2\text{OZn}$: C 29.98, H 3.72, N 5.19%.

Crystal data

$[\text{ZnBr}_2(\text{C}_{13}\text{H}_{19}\text{BrN}_2\text{O})]$	$D_x = 1.969 \text{ Mg m}^{-3}$
$M_r = 524.40$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 2246 reflections
$a = 7.147 (1) \text{ \AA}$	$\theta = 2.4\text{--}25.3^\circ$
$b = 15.722 (2) \text{ \AA}$	$\mu = 8.16 \text{ mm}^{-1}$
$c = 16.077 (3) \text{ \AA}$	$T = 298 (2) \text{ K}$
$\beta = 101.768 (2)^\circ$	Block, colourless
$V = 1768.5 (5) \text{ \AA}^3$	$0.17 \times 0.15 \times 0.15 \text{ mm}$
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	4003 independent reflections
ω scans	2209 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.088$
$T_{\text{min}} = 0.265$, $T_{\text{max}} = 0.294$	$\theta_{\text{max}} = 27.5^\circ$
14691 measured reflections	$h = -9 \rightarrow 9$
	$k = -19 \rightarrow 20$
	$l = -20 \rightarrow 20$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.053$	$w = 1/[\sigma^2(F_o^2) + (0.056P)^2]$
$wR(F^2) = 0.139$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{\text{max}} < 0.001$
4003 reflections	$\Delta\rho_{\text{max}} = 0.93 \text{ e \AA}^{-3}$
186 parameters	$\Delta\rho_{\text{min}} = -0.76 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

Zn1—O1	1.915 (5)	Zn1—Br2	2.3399 (14)
Zn1—N1	2.021 (5)	Zn1—Br3	2.4517 (13)
O1—Zn1—N1	96.0 (2)	O1—Zn1—Br3	109.01 (15)
O1—Zn1—Br2	119.66 (14)	N1—Zn1—Br3	104.66 (15)
N1—Zn1—Br2	115.13 (16)	Br2—Zn1—Br3	110.64 (5)

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$D\text{—}H\cdots A$	$D\text{—}H$	$H\cdots A$	$D\cdots A$	$D\text{—}H\cdots A$
$\text{N2—H2}\cdots\text{Br3}$	0.90 (6)	2.67 (6)	3.375 (5)	136 (7)

Atom H2, bonded to N2, was located in a difference Fourier map and refined isotropically, with the N—H distance restrained to 0.90 (1) \AA . All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93–0.97 \AA and $U_{\text{iso}}(\text{H}) = 1.2$ or $1.5U_{\text{eq}}(\text{C})$.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

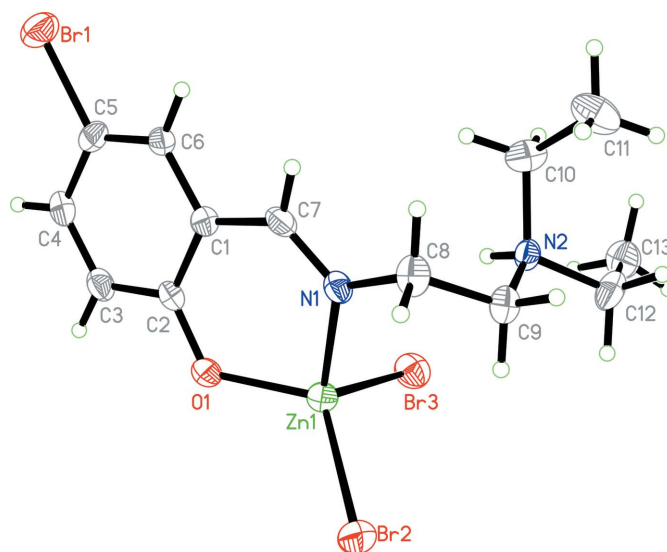


Figure 1

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

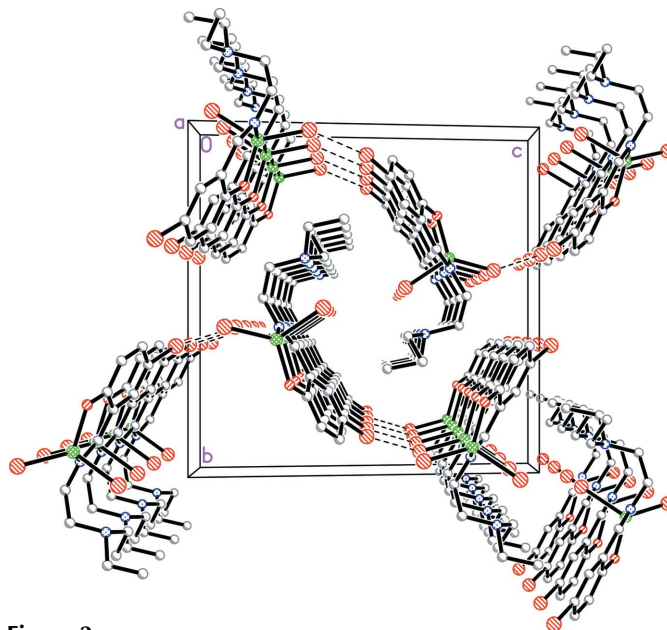


Figure 2

The crystal packing of (I), viewed along the a axis. Weak Br \cdots Br interactions are shown as dashed lines.

This work was supported by the Scientific Research Foundation of the Education Office of Liaoning Province (project No. 2005226).

References

- Archer, R. D. & Wang, B. (1990). *Inorg. Chem.* **29**, 39–43.
 Bhatia, S. C., Bindlish, J. M., Saini, A. R. & Jain, P. C. (1981). *J. Chem. Soc. Dalton Trans.* pp. 1773–1779.
 Bruker (1998). SMART (Version 5.628) and SAINT (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
 Chang, S., Jones, L., Wang, C. M., Henling, L. M. & Grubbs, R. H. (1998). *Organometallics*, **17**, 3460–3465.
 Chaturvedi, K. K. (1977). *J. Inorg. Nucl. Chem.* **39**, 901–903.
 Ciurli, S., Benini, S., Rypniewski, W. R., Wilson, K. S., Miletto, S. & Mangani, S. (1999). *Coord. Chem. Rev.* **190–192**, 331–335.

- Costamagna, J., Vargas, J., Latorre, R., Alvarado, A. & Mena, G. (1992). *Coord. Chem. Rev.* **119**, 67–88.
- Park, I.-S. & Hausinger, R. P. (1996). *Biochemistry*, **35**, 5345–5352.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997a). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997b). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
- Yamada, S. (1999). *Coord. Chem. Rev.* **190–192**, 537–555.
- You, Z.-L. (2005a). *Acta Cryst.* **E61**, m1571–m1573.
- You, Z.-L. (2005b). *Acta Cryst.* **C61**, m456–m458.
- You, Z.-L. (2005c). *Acta Cryst.* **C61**, m383–m385.