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Dibromo{2-[2-(ethylamino)ethyliminomethyl]-4-nitrophenolato}zinc(II)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.036
wR factor = 0.087
Data-to-parameter ratio = 20.1

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

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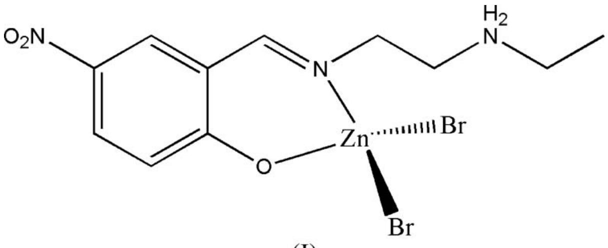
In the title mononuclear zinc(II) complex, [ZnBr$_2$-(C$_{11}$H$_{15}$N$_3$O$_3$)], the Zn atom is four-coordinated in a tetrahedral configuration by one imine N and one phenolate O atoms of the Schiff base ligand, and by two terminal Br atoms. In the crystal structure, molecules are linked through intermolecular N—H···O, N—H···Br, C—H···O and C—H···Br hydrogen bonds, forming a three-dimensional network.

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 have played an important role in the development of coordination chemistry related to catalysis and enzymatic reactions, magnetism and molecular architectures (Costamagna *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; You *et al.*, 2006). As an extension of the work on these complexes, the title zinc(II) complex, (I), is reported here.



(I)

Compound (I) is a mononuclear zinc(II) complex (Fig. 1). The Zn 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 other Schiff base–zinc(II) complexes (Ma, Lv *et al.*, 2006; Ma, Gu *et al.*, 2006) and those cited above. The conformation of the N1–C11 chain is a mixture of *gauche* and *anti* segments. There is an intramolecular N—H···Br hydrogen bond (Table 2) in the complex.

In the crystal structure, molecules are linked through intermolecular N—H···O, N—H···Br, C—H···O and C—H···Br hydrogen bonds (Table 2), forming a three-dimensional network (Fig. 2).

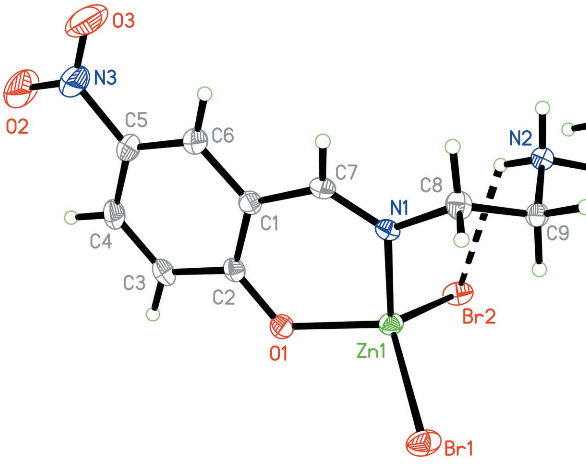


Figure 1
View of the molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. The intramolecular N—H⋯Br hydrogen bond is shown as a dashed line.

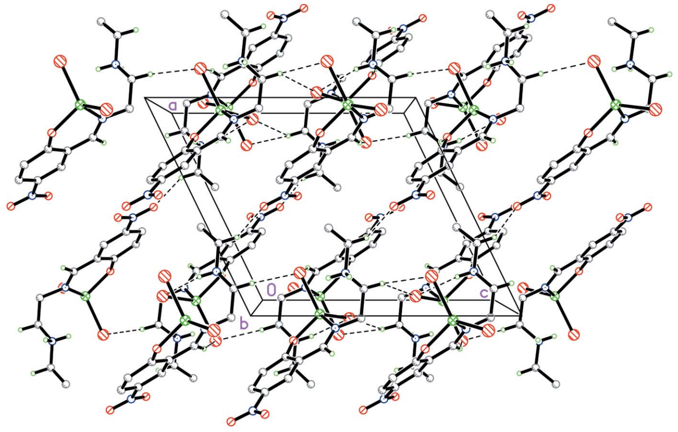


Figure 2
The crystal packing of (I), viewed along the *b* axis. Intermolecular hydrogen bonds are shown as dashed lines.

Experimental

N-Ethylethane-1,2-diamine and 5-nitrosalicylaldehyde were available commercially and were used without further purification. *N*-Ethylethane-1,2-diamine (0.1 mmol, 8.8 mg) and 5-nitrosalicylaldehyde (0.1 mmol, 16.7 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 a further 30 min at room temperature, giving a clear colourless solution. After allowing the solution to stand in air for a week, colourless block-shaped crystals were formed on slow evaporation of the solvent. Analysis found: C 28.39, H 3.38, N 9.20%; calculated for $C_{11}H_{15}Br_2N_3O_3Zn$: C 28.57, H 3.27, N 9.09%.

Crystal data

$[ZnBr_2(C_{11}H_{15}N_3O_3)]$
$M_r = 462.45$
Monoclinic, $P2_1/c$
$a = 11.714$ (2) Å
$b = 11.683$ (2) Å
$c = 13.070$ (2) Å
$\beta = 115.912$ (3)°
$V = 1608.9$ (5) Å^3
$Z = 4$
$D_x = 1.909$ Mg m^{-3}
Mo *Kα* radiation
$\mu = 6.50$ mm^{-1}
$T = 298$ (2) K
Block, colourless
0.24 × 0.23 × 0.21 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.228$, $T_{max} = 0.257$
13397 measured reflections
3659 independent reflections
2633 reflections with $I > 2\sigma(I)$
$R_{int} = 0.052$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.088$
$S = 1.02$
3659 reflections
182 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0236P)^2 + 1.0083P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.55$ e Å^{-3}
$\Delta\rho_{min} = -0.88$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.954 (3)	Zn1—Br1	2.3428 (7)
Zn1—N1	1.997 (3)	Zn1—Br2	2.3828 (8)
O1—Zn1—N1	97.25 (11)	O1—Zn1—Br2	109.84 (9)
O1—Zn1—Br1	107.91 (8)	N1—Zn1—Br2	110.57 (8)
N1—Zn1—Br1	109.87 (8)	Br1—Zn1—Br2	119.14 (2)

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

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
N2—H2*B*⋯O1^{i}	0.90	2.03	2.903 (4)	164
N2—H2*A*⋯Br1^{i}	0.90	2.71	3.416 (3)	137
N2—H2*A*⋯Br2	0.90	2.87	3.503 (3)	128
C7—H7⋯Br2^{i}	0.93	2.84	3.699 (3)	153
C9—H9*A*⋯Br2^{ii}	0.97	2.91	3.822 (4)	157
C10—H10*B*⋯O2^{iii}	0.97	2.43	3.262 (6)	144

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

H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93–0.97 Å and $U_{iso}(H) = 1.2$ or $1.5U_{eq}(C)$.

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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