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Key indicators

Single-crystal X-ray study
 T = 298 K
 Mean $\sigma(C-C)$ = 0.005 Å
 R factor = 0.033
 wR factor = 0.094
 Data-to-parameter ratio = 14.8

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

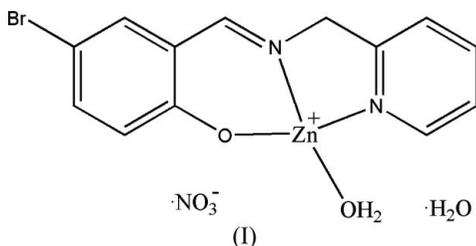
Aqua[4-bromo-2-(pyridinylmethylimino-methyl)phenolato]zinc(II) nitrate monohydrate

In the cation of the title complex, $[Zn(C_{13}H_{10}BrN_2O)(H_2O)](NO_3) \cdot H_2O$, the Zn atom is coordinated by two N and two O atoms, giving a slightly distorted square-planar geometry. The crystal structure is stabilized by intermolecular O—H...O hydrogen-bond interactions.

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Comment

The Zn^{II} cation permits a wide variety of coordination geometry (Erxleben, 2001; Chisholm *et al.*, 2001; Halvorsen *et al.*, 1995; Brand & Vahrenkamp, 2000). The Schiff base ligand 4-bromo-2-(pyridinylmethyliminomethyl)phenol is a tridentate chelating agent. However, this ligand does not saturate the coordination of Zn, which is thus potentially suitable to be coordinated by other donor atoms. A new zinc(II) complex, (I), derived from the tridentate chelating Schiff base ligand, is described here.



The crystal structure of (I) is shown in Fig. 1. The complex consists of a mononuclear zinc(II) cation, a nitrate anion and an uncoordinated water molecule. In the cation, the coord-

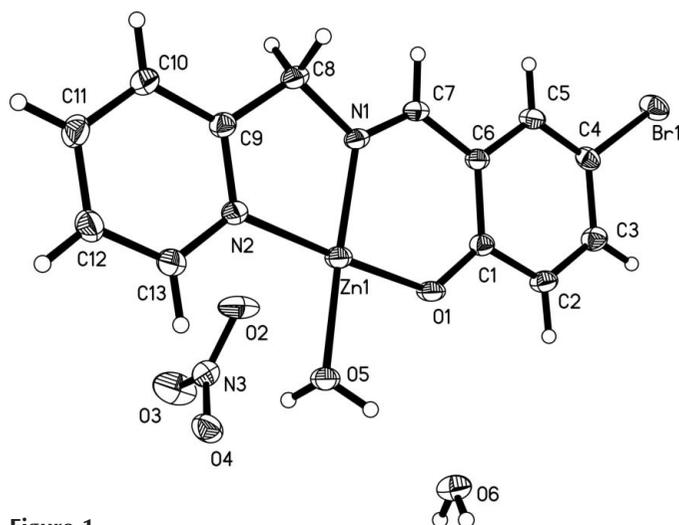


Figure 1 The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

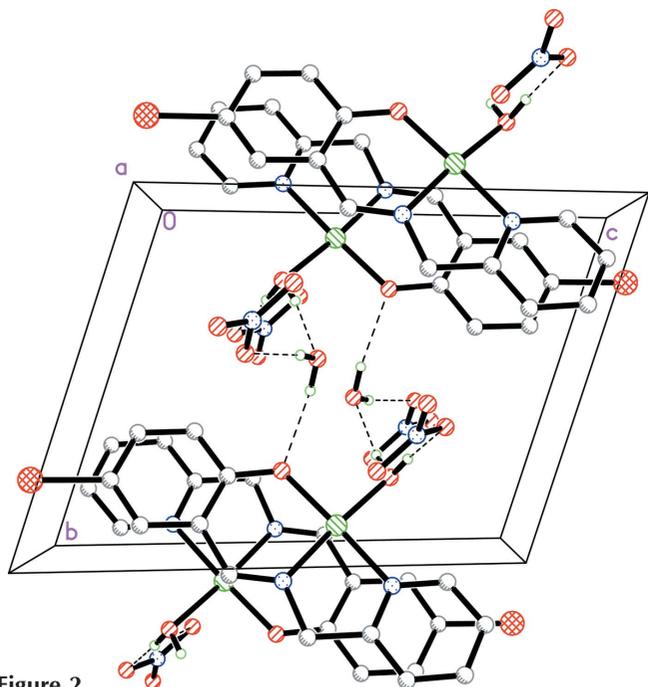


Figure 2
The packing of (I); the dashed lines indicate intermolecular O—H...O hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted.

ination sites are occupied by the donor atoms of the Schiff base ligand and by the O atom of a water molecule, giving a slightly distorted square-planar geometry with an average deviation of 0.075 (3) Å; the Zn atom lies 0.0642 (4) Å above this plane. The Schiff base ligand is nearly planar with an average deviation of 0.035 (2) Å. The Zn1—N2 distance (Table 1) is appreciably longer than the Zn1—N1 bond distance because of the steric requirements of the rigid Schiff base ligand.

The crystal packing of (I) is shown in Fig. 2. There are intermolecular O—H...O hydrogen-bond interactions (Table 2) stabilizing the structure.

Experimental

All the chemicals were of AR grade. 5-Bromosalicylaldehyde (40.2 mg, 0.2 mmol) and 2-aminomethylpyridine (21.6 mg, 0.2 mmol) were refluxed in 10 ml methanol for 30 min, then an aqueous solution (10 ml) of $\text{Zn}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (58.6 mg, 0.2 mmol) was added. The mixture was refluxed for 1 h. The mixture was cooled to room temperature and filtered. After keeping the filtrate in air for 3 d, yellow block crystals suitable for X-ray analysis were obtained.

Crystal data

$[\text{Zn}(\text{C}_{13}\text{H}_{10}\text{BrN}_2\text{O})(\text{H}_2\text{O})](\text{NO}_3) \cdot \text{H}_2\text{O}$
 $M_r = 453.55$
 Triclinic, $P\bar{1}$
 $a = 7.841$ (2) Å
 $b = 9.043$ (2) Å
 $c = 12.012$ (2) Å
 $\alpha = 106.962$ (2)°
 $\beta = 102.781$ (3)°
 $\gamma = 93.040$ (3)°
 $V = 788.2$ (3) Å³

$Z = 2$
 $D_x = 1.911$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 3326 reflections
 $\theta = 2.5$ – 27.8 °
 $\mu = 4.13$ mm⁻¹
 $T = 298$ (2) K
 Block, yellow
 $0.18 \times 0.13 \times 0.10$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2000)
 $T_{\min} = 0.508$, $T_{\max} = 0.662$
 6664 measured reflections

3390 independent reflections
 2901 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.018$
 $\theta_{\max} = 27.0$ °
 $h = -9 \rightarrow 10$
 $k = -11 \rightarrow 11$
 $l = -15 \rightarrow 15$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.094$
 $S = 1.04$
 3390 reflections
 229 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0513P)^2 + 0.5173P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.85$ e Å⁻³
 $\Delta\rho_{\min} = -0.45$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Zn1—O1	1.890 (2)	Zn1—O5	1.979 (2)
Zn1—N1	1.937 (2)	Zn1—N2	1.983 (2)
O1—Zn1—N1	93.63 (9)	O1—Zn1—N2	176.84 (9)
O1—Zn1—O5	88.94 (9)	N1—Zn1—N2	83.32 (10)
N1—Zn1—O5	171.43 (10)	O5—Zn1—N2	94.20 (9)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O6—H6A...O1 ⁱ	0.85 (3)	2.10 (3)	2.929 (3)	168 (4)
O5—H5B...O6	0.84 (4)	1.83 (4)	2.659 (3)	168 (4)
O5—H5C...O4	0.84 (4)	1.83 (4)	2.664 (3)	172 (4)
O6—H6B...O3 ⁱⁱ	0.85 (4)	1.95 (4)	2.780 (4)	167 (4)

Symmetry codes: (i) $-x + 1, -y + 1, -z + 1$; (ii) $x + 1, y, z$.

H atoms of the water molecules were located in a difference Fourier map and refined isotropically, with O—H distances restrained to 0.85 (1) Å and H...H distances restrained to 1.38 (2) Å. All other H atoms were positioned geometrically and refined as riding atoms, with C—H distances of 0.93–0.97 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Bruker, 2000); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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