

## Aqua[2-(pyridin-2-ylmethyliminomethyl)-phenolato]zinc(II) nitrate monohydrate

Zong-Xiao Li and Xin-Li Zhang\*

Department of Chemistry and Chemical  
Engineering, Baoji College of Arts and Sciences,  
Baoji 721007, People's Republic of ChinaCorrespondence e-mail:  
baojizhangxinli@163.com

## Key indicators

Single-crystal X-ray study  
 $T = 298\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$   
 $R$  factor = 0.045  
 $wR$  factor = 0.131  
Data-to-parameter ratio = 13.5For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

In the crystal structure of the title compound,  $[\text{Zn}(\text{C}_{13}\text{H}_{11}\text{N}_2\text{O})(\text{H}_2\text{O})](\text{NO}_3)\cdot\text{H}_2\text{O}$ , the Zn atom is coordinated by two N atoms and one O atom from the Schiff base ligand, and another O atom from a water molecule. The four atoms around the metal constitute a slightly distorted square-planar geometry. The O atoms in both the ions and water molecules contribute to O—H $\cdots$ O hydrogen bonds, leading to the formation of sheets parallel to the *ac* and *bc* planes.

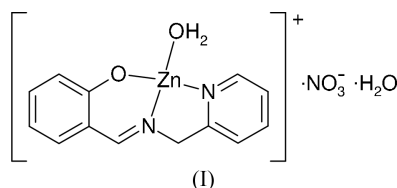
Received 7 June 2004

Accepted 23 June 2004

Online 30 June 2004

## Comment

Transition metal compounds containing Schiff base ligands have been of great interest for many years. These compounds play 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). As an extension of the work on the structural characterization of Schiff base complexes, the crystal structure of a mononuclear zinc(II) compound, (I), is reported here.



The asymmetric unit of (I) (Fig. 1), consists of a mononuclear  $[\text{Zn}(\text{C}_{13}\text{H}_{11}\text{N}_2\text{O})(\text{H}_2\text{O})]^+$  cation, a nitrate anion and an uncoordinated water molecule. The Zn atom is in a square-

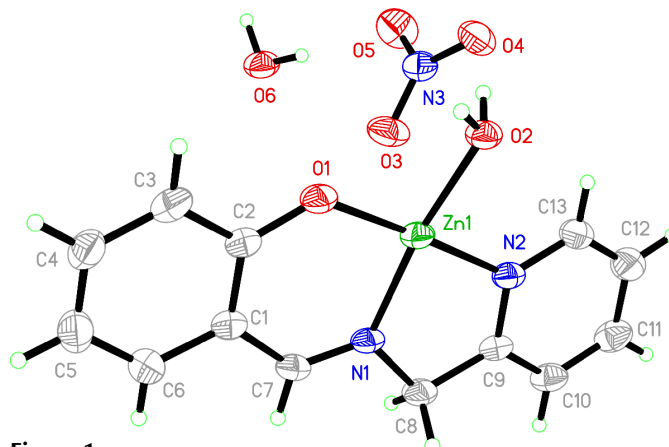
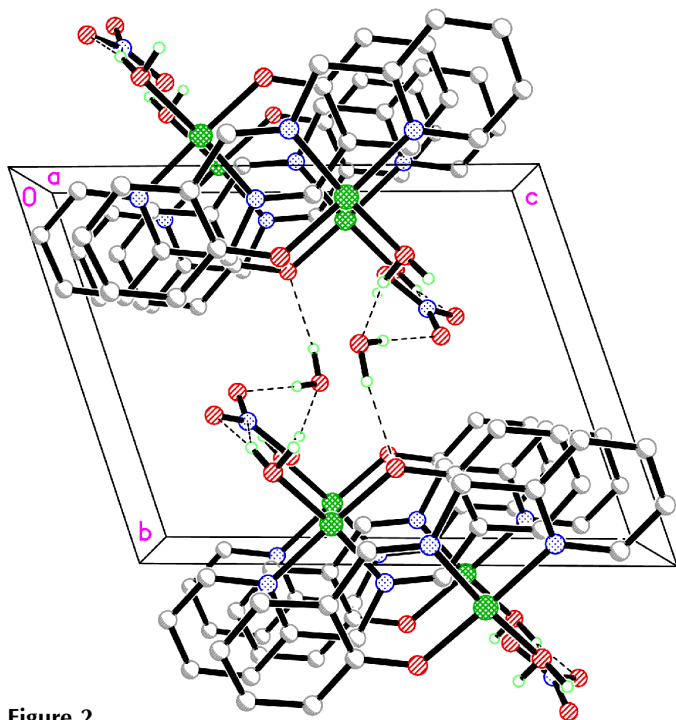


Figure 1

The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.



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

planar geometry and is four-coordinated by one O atom and two N atoms from the Schiff base ligand, and one O atom from a water molecule. The four coordinating atoms around Zn are approximately coplanar, giving a square-planar geometry with an average deviation of 0.090 (4) Å, the Zn atom being 0.063 (2) Å above this plane.

The C7=N1 bond distance of 1.283 (4) Å conforms to the value for a double bond, while the C8–N1 bond distance of 1.469 (4) Å conforms to the value for a single bond. The Zn1–O1 bond length of 1.892 (2) Å (Table 1) is a little shorter than the value of 1.977 (2) Å observed in another Schiff base complex (Ülkü *et al.*, 2000). The Zn1–N1 bond distance of 1.927 (2) Å is also a little shorter than the value of 2.058 (3) Å observed in yet another Schiff base zinc(II) compound (Tatar *et al.*, 2002). The Zn1–N2 and Zn1–O2 distances are comparable with the values found in most zinc(II) compounds (Blake *et al.*, 2001). The bond angles around the Zn<sup>II</sup> center show some deviations from ideal square-planar geometry. All the O atoms in the nitrate anions, the water molecules and the 2-aminomethylpyridine ligand contribute to O–H···O hydrogen bonds, leading to the formation of sheets parallel to the *ac* and *bc* planes (Table 2 and Fig. 2).

## Experimental

All chemicals used (reagent grade) were commercially available. 2-Aminomethylpyridine (0.1 mmol, 10.8 mg) and Zn(CH<sub>3</sub>COO)<sub>2</sub>·2H<sub>2</sub>O (0.1 mmol, 22.0 mg) were dissolved in ethanol (10 ml). The mixture was stirred for 30 min to give a clear colorless solution, which was allowed to evaporate slowly in the air at room temperature. After 21 d, colorless block-shaped crystals of (I) were formed at the bottom

of the vessel. These crystals were isolated, washed three times with ethanol and dried in a vacuum desiccator using anhydrous CaCl<sub>2</sub> (yield 54.9%). Analysis found: C 41.5, H 4.1, N 11.3%; calculated for C<sub>13</sub>H<sub>15</sub>N<sub>3</sub>O<sub>6</sub>Zn: C 41.7, H 4.0, N 11.2%.

### Crystal data

[Zn(C <sub>13</sub> H <sub>11</sub> N <sub>2</sub> O)(H <sub>2</sub> O)](NO <sub>3</sub> )·H <sub>2</sub> O	Z = 2
<i>M<sub>r</sub></i> = 374.65	<i>D<sub>x</sub></i> = 1.655 Mg m <sup>-3</sup>
Triclinic, <i>P</i> $\bar{1}$	Mo <i>K</i> α radiation
<i>a</i> = 7.7746 (7) Å	Cell parameters from 2203 reflections
<i>b</i> = 8.9911 (8) Å	<i>θ</i> = 2.4–26.7°
<i>c</i> = 11.3884 (10) Å	<i>μ</i> = 1.67 mm <sup>-1</sup>
<i>α</i> = 71.226 (1)°	<i>T</i> = 298 (2) K
<i>β</i> = 86.229 (1)°	Block, colorless
<i>γ</i> = 86.914 (1)°	0.22 × 0.18 × 0.15 mm
<i>V</i> = 751.64 (12) Å <sup>3</sup>	

### Data collection

Bruker SMART CCD area-detector diffractometer	3024 independent reflections
<i>ω</i> scans	2534 reflections with <i>I</i> > 2σ( <i>I</i> )
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	<i>R<sub>int</sub></i> = 0.020
<i>T<sub>min</sub></i> = 0.710, <i>T<sub>max</sub></i> = 0.788	<i>θ<sub>max</sub></i> = 26.5°
5888 measured reflections	<i>h</i> = -9 → 9
	<i>k</i> = -11 → 11
	<i>l</i> = -14 → 14

### Refinement

Refinement on <i>F</i> <sup>2</sup>	<i>w</i> = 1/[σ <sup>2</sup> ( <i>F<sub>o</sub></i> <sup>2</sup> ) + (0.0821 <i>P</i> ) <sup>2</sup> + 0.0976 <i>P</i> ]
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )] = 0.045	where <i>P</i> = ( <i>F<sub>o</sub></i> <sup>2</sup> + 2 <i>F<sub>c</sub></i> <sup>2</sup> )/3
<i>wR</i> ( <i>F</i> <sup>2</sup> ) = 0.131	(Δσ) <sub>max</sub> < 0.001
<i>S</i> = 1.07	Δρ <sub>max</sub> = 0.63 e Å <sup>-3</sup>
3024 reflections	Δρ <sub>min</sub> = -0.28 e Å <sup>-3</sup>
224 parameters	
H atoms treated by a mixture of independent and constrained refinement	

**Table 1**

Selected geometric parameters (Å, °).

Zn1–O1	1.892 (2)	Zn1–O2	1.975 (2)
Zn1–N1	1.927 (2)	Zn1–N2	1.990 (3)
O1–Zn1–N1	94.15 (11)	O1–Zn1–N2	176.24 (10)
O1–Zn1–O2	89.03 (10)	N1–Zn1–N2	82.55 (11)
N1–Zn1–O2	170.50 (10)	O2–Zn1–N2	94.51 (11)

**Table 2**

Hydrogen-bonding geometry (Å, °).

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
O2–H2A···O4	0.896 (10)	1.810 (14)	2.683 (4)	164 (4)
O2–H2A···N3	0.896 (10)	2.52 (3)	3.252 (4)	139 (4)
O2–H2A···O3	0.896 (10)	2.58 (4)	3.024 (4)	111 (3)
O6–H6A···O5	0.894 (10)	1.932 (12)	2.819 (4)	172 (3)
O2–H2B···O6 <sup>i</sup>	0.892 (10)	1.787 (14)	2.661 (3)	166 (3)
O6–H6B···O1 <sup>ii</sup>	0.902 (10)	2.024 (14)	2.911 (3)	168 (3)

Symmetry codes: (i) *x* – 1, *y*, *z*; (ii) 1 – *x*, 1 – *y*, 1 – *z*.

Water H atoms were located in a difference Fourier map and refined isotropically, with the O–H and H···H distances restrained to 0.89 (1) and 1.43 (1) Å, respectively. All remaining 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*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C). The highest peak in the final difference map was located 0.48 Å from atom H5A.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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*.

The authors thank Baoji College of Arts and Sciences for a research grant.

## References

- Bhatia, S. C., Bindlish, J. M., Saini, A. R. & Jain, P. C. (1981). *J. Chem. Soc. Dalton Trans.* pp. 1773–1779.
- Blake, A. J., Cooke, P. A., Hubberstey, P. & Sampson, C. L. (2001). *Acta Cryst. E57*, i109–i111.
- Costamagna, J., Vargas, J., Latorre, R., Alvarado, A. & Mena, G. (1992). *Coord. Chem. Rev.* **119**, 67–88.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
- Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
- Tatar, L., Atakol, O. & Ülkü, D. (2002). *Acta Cryst. E58*, m83–m85.
- Ülkü, D., Arici, C. Tahir, M. N. & Atakol, O. (2000). *Acta Cryst. C56*, 1298–1299.