

Hua-Jie Xu, Zhao-Di Liu and
Liang-Quan Sheng*Department of Chemistry, Fuyang Normal
College, Fuyang Anhui 236041, People's
Republic of China

Correspondence e-mail: shenglq@fync.edu.cn

***trans*-Bis{2-[(4-hydroxyphenethylimino)-
methyl]phenolato}zinc(II) monohydrate**

The title compound, $[\text{Zn}(\text{C}_{15}\text{H}_{14}\text{NO}_2)_2]\cdot\text{H}_2\text{O}$, is a mononuclear zinc(II) compound. The Zn^{II} atom, located on an inversion centre, is coordinated by two N atoms and two O atoms from two Schiff base ligands in a square-planar geometry. The $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonding involving the water molecules located on a twofold axis links the complex molecules into a three-dimensional network.

Received 12 September 2006

Accepted 16 September 2006

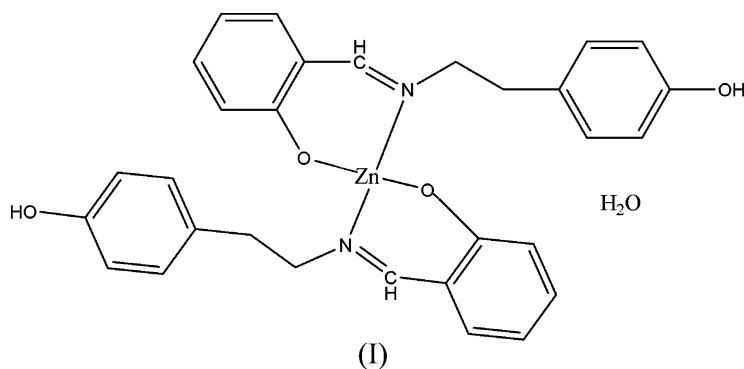
Key indicators

Single-crystal X-ray study
 $T = 292\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$
 R factor = 0.054
 wR factor = 0.161
Data-to-parameter ratio = 18.1

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

Comment

Transition metal compounds containing Schiff base ligands have been of great interest for many years (Asada *et al.*, 2003; Zhu *et al.*, 2000; Yamada, 1999; Archer & Wang, 1990). 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). Zinc has long been recognized as an important cofactor in biological molecules, either as a structural template in protein folding or as a Lewis acid catalyst that can readily adopt four-, five- or six-coordination (Vallee & Auld, 1993; You *et al.*, 2003; You, Ma *et al.*, 2004; You, Zhu *et al.*, 2004). The crystal structure of a mononuclear zinc(II) compound, (I), is reported here.



The asymmetric unit of (I) consists of half each of an electronically neutral mononuclear Zn^{II} complex and a water molecule (Fig. 1). Atom Zn1 of the complex molecule lies on an inversion centre, while the water atom O1W lies on a twofold axis. The Zn^{II} ion in the compound is four-coordinated by two O atoms and two N atoms from two Schiff base ligands. This CuO_2N_2 coordination forms a square-planar geometry.

In the crystal structure, the O atoms of the Schiff base ligands and the water molecules contribute to hydrogen bonds, leading to the formation of a three-dimensional network (Fig. 2).

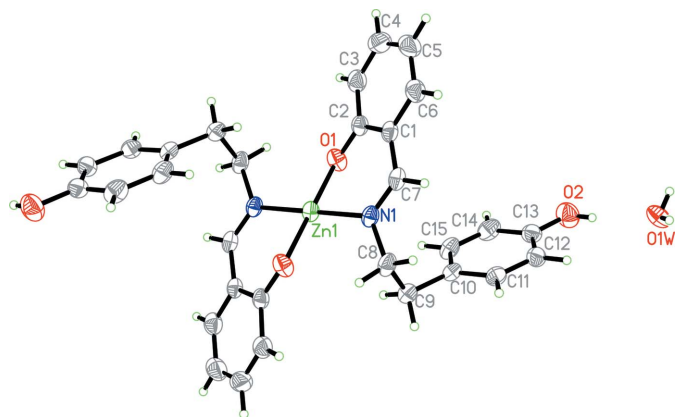


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. Unlabelled atoms are related to labelled atoms by the symmetry operator $(1 - x, 2 - y, 1 - z)$.

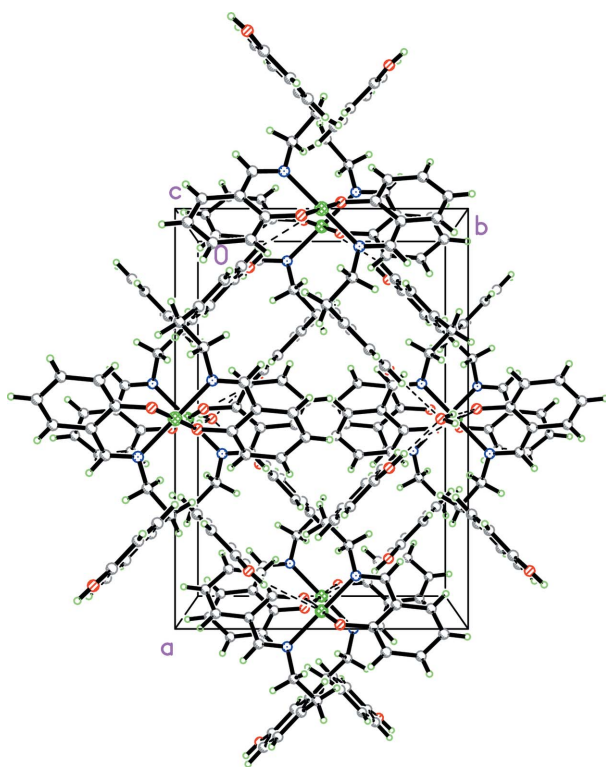


Figure 2
The crystal packing of (I), viewed along the c axis. Dashed lines indicate hydrogen bonds.

Experimental

4-(2-Aminoethyl)phenol and salicylaldehyde were available commercially and were used without further purification. 4-(2-Aminoethyl)phenol (0.2 mmol, 27.8 mg) and salicylaldehyde (0.2 mmol, 24.4 mg) were dissolved in methanol (15 ml) and the mixture was stirred for 1 h to give a clear orange solution of L (0.2 mmol), where L is 2-[4-hydroxyphenethylimino)methyl]phenol. To the solution of L was added a methanol solution (10 ml) of $ZnCl_2$ (0.1 mmol, 13.6 mg) with stirring. After keeping the resulting solution at room temperature in air for 14 d, colourless block-shaped crystals

were formed at the bottom of the vessel on slow evaporation of the solvent. The crystals were isolated, washed with ethanol and dried.

Crystal data

$[Zn(C_{15}H_{14}NO_2)_2] \cdot H_2O$
 $M_r = 563.93$
Orthorhombic, $Pbcn$
 $a = 15.533(3) \text{ \AA}$
 $b = 10.822(2) \text{ \AA}$
 $c = 16.003(3) \text{ \AA}$
 $V = 2690.0(9) \text{ \AA}^3$

$Z = 4$
 $D_x = 1.392 \text{ Mg m}^{-3}$
Mo $K\alpha$ radiation
 $\mu = 0.96 \text{ mm}^{-1}$
 $T = 292(2) \text{ K}$
Block, colourless
 $0.36 \times 0.20 \times 0.13 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.725, T_{\max} = 0.886$

20847 measured reflections
3221 independent reflections
1811 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.099$
 $\theta_{\text{max}} = 27.5^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.054$
 $wR(F^2) = 0.161$
 $S = 0.92$
3221 reflections
178 parameters

H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0907P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.76 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.64 \text{ e \AA}^{-3}$

Table 1

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

Zn1—O1	1.907 (2)	Zn1—N1	2.001 (3)
O1 ⁱ —Zn1—O1	180	O1—Zn1—N1	89.93 (10)
O1—Zn1—N1 ⁱ	90.07 (10)	N1 ⁱ —Zn1—N1	180

Symmetry code: (i) $-x + 1, -y + 2, -z + 1$.

Table 2

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

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O2—H2 \cdots O1W	0.82	1.97	2.776 (4)	167
O1W—H1WA \cdots O1 ⁱⁱ	0.84 (1)	1.95 (2)	2.776 (3)	173 (3)

Symmetry code: (ii) $x - \frac{1}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$.

The water H atom was located in a difference map and refined with O—H and H \cdots H distance restraints of 0.84 (1) and 1.37 (2) \AA , respectively. The remaining H atoms were placed in idealized positions (O—H = 0.82 \AA , and C—H = 0.93 or 0.97 \AA) and constrained to ride on their parent atoms with $U_{\text{iso}}(\text{H})$ values of 1.2 or 1.5 (hydroxy) times $U_{\text{eq}}(\text{C}, \text{O})$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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: *SHELXL97*.

This work was supported by the Natural Science Foundation of Anhui Provincial University College (grant No. 2006 K

J125B) and Fuyang Normal College, China (grant No. 2005LQ06).

References

- Archer, R. D. & Wang, B. (1990). *Inorg. Chem.* **29**, 39–43.
- Asada, H., Hayashi, K., Negoro, S., Fujiwara, M. & Matsushita, T. (2003). *Inorg. Chem. Commun.* **6**, 193–196.
- Bhatia, S. C., Bindlish, J. M., Saini, A. R. & Jain, P. C. (1981). *J. Chem. Soc. Dalton Trans.* pp. 1773–1779.
- 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. (1997a). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997b). *SHELXTL*. Version. 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
- Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
- Vallee, B. L. & Auld, D. S. (1993). *Acc. Chem. Res.* **26**, 543–551.
- Yamada, S. (1999). *Coord. Chem. Rev.* **190–192**, 537–555.
- You, Z.-L., Lin, Y.-S., Liu, W.-S., Tan, M.-Y. & Zhu, H.-L. (2003). *Acta Cryst. E59*, m1025–m1027.
- You, Z.-L., Ma, J.-L., Zhu, H.-L. & Liu, W.-S. (2004). *Acta Cryst. E60*, m1599–m1601.
- You, Z.-L., Zhu, H.-L. & Liu, W.-S. (2004). *Acta Cryst. E60*, m560–m562.
- Zhu, H.-L., Tong, Y.-X. & Chen, X.-M. (2000). *J. Chem. Soc. Dalton Trans.* pp. 4182–4186.