

San-Jun Peng,^{a*} Cong-Shan
Zhou^b and Tao Yang^b^aDepartment of Chemistry and Environmental Engineering, Changsha University of Science and Technology, Changsha 410076, People's Republic of China, and ^bDepartment of Chemistry and Chemical Engineering, Hunan Institute of Science and Technology, Yueyang 414006, People's Republic of China

Correspondence e-mail: sanjunpeng@163.com

Key indicators

Single-crystal X-ray study
 $T = 298\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$
 R factor = 0.030
 wR factor = 0.080
Data-to-parameter ratio = 20.3For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

Dichloro{2-[2-(ethylamino)ethylimino-methyl]phenolato}zinc(II)

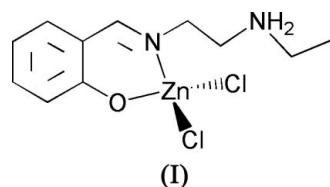
In the title mononuclear zinc(II) complex, $[\text{ZnCl}_2(\text{C}_{11}\text{H}_{16}\text{N}_2\text{O})]$, the Zn^{II} atom is coordinated by the imine N and phenolate O atoms of the Schiff base ligand and two chloride anions to give a four-coordinate tetrahedral geometry. In the crystal structure, the molecules are linked through intermolecular $\text{N}-\text{H}\cdots\text{O}$, $\text{N}-\text{H}\cdots\text{Cl}$ and $\text{C}-\text{H}\cdots\text{Cl}$ hydrogen bonds, forming layers parallel to the ab plane.

Received 21 April 2006

Accepted 23 April 2006

Comment

Zinc is the second most abundant transition or post-transition metal in biology. It functions as the active site of hydrolytic enzymes, such as carboxypeptidase and carbonic anhydrase, where it is in a hard-donor coordination environment of nitrogen and oxygen (Lipscomb & Sträter, 1996; Bertini *et al.*, 1994). It also 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 (Harrison *et al.*, 2006; Tirosh *et al.*, 2005; Musie *et al.*, 2004; Vallee & Auld, 1993). Recent reports have suggested that zinc is able to play a catalytic role in the activation of thiols as nucleophiles at physiological pH (Wilker & Lippard, 1997; Myers *et al.*, 1993). We have reported the structures of a number of transition metal complexes (Peng *et al.*, 2005, 2006) and report here the structure of a new tetrahedral zinc(II) complex, (I), derived from 2-[2-(ethylamino)ethyliminomethyl]phenol.



The Zn^{II} atom in (I) is coordinated by the imine N and phenolate O atoms of the Schiff base ligand and by two chloride anions, forming a tetrahedral geometry (Fig. 1). As expected, the C8/C9/N2/C10/C11 unit adopts a zigzag geometry to minimize steric effects. The amine N atom is protonated and does not coordinate to the metal ion. The $\text{Zn}-\text{O}$ and $\text{Zn}-\text{N}$ bond lengths (Table 1) are comparable to the values in other similar complexes (Qiu, 2006; You *et al.*, 2006; You, 2006; Tatar, Atakol & Arici, 2002; Tatar, Atakol & Ülkü, 2002; Ülkü *et al.*, 2000). The angles subtended at the Zn atom range from $96.84(7)$ to $115.04(3)^\circ$ (Table 1), indicating a distorted tetrahedral coordination for the metal ion.

In the crystal structure, the molecules are linked through intermolecular N—H···O, N—H···Cl and C—H···Cl hydrogen bonds (Table 2), forming layers parallel to the *ab* plane, as shown in Fig. 2.

Experimental

Salicylaldehyde (0.5 mmol, 61.1 mg) and *N*-ethylethane-1,2-diamine (0.5 mmol, 44.1 mg) were stirred into 30 ml of methanol. After 1 h, ZnCl₂ (0.3 mmol, 51.0 mg) in methanol (10 ml) was added, and the stirring continued for a further 1 h. The filtrate was kept at room temperature for about a week, depositing colourless block-shaped crystals of (I). Analysis found: C 40.03, H 4.82, N 8.60%; calculated for C₁₁H₁₆Cl₂N₂OZn: C 40.21, H 4.91, N 8.53%.

Crystal data

[ZnCl ₂ (C ₁₁ H ₁₆ N ₂ O)]	Z = 4
<i>M_r</i> = 328.53	<i>D_x</i> = 1.580 Mg m ⁻³
Monoclinic, <i>P</i> 2 ₁ / <i>n</i>	Mo <i>K</i> α radiation
<i>a</i> = 7.406 (1) Å	<i>μ</i> = 2.15 mm ⁻¹
<i>b</i> = 11.770 (1) Å	<i>T</i> = 298 (2) K
<i>c</i> = 16.123 (1) Å	Block, colourless
<i>β</i> = 100.606 (1)°	0.25 × 0.22 × 0.18 mm
<i>V</i> = 1381.4 (2) Å ³	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	11598 measured reflections
<i>ω</i> scans	3140 independent reflections
Absorption correction: multi-scan (<i>SADABS</i> ; Bruker, 2000)	2700 reflections with <i>I</i> > 2σ(<i>I</i>)
<i>T_{min}</i> = 0.616, <i>T_{max}</i> = 0.698	<i>R_{int}</i> = 0.020
	<i>θ_{max}</i> = 27.5°

Refinement

Refinement on <i>F</i> ²	$w = 1/[\sigma^2(F_o^2) + (0.0432P)^2 + 0.4581P]$
$R[F^2 > 2\sigma(F^2)] = 0.030$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.080$	(Δ/σ) _{max} < 0.001
<i>S</i> = 1.03	$\Delta\rho_{max} = 0.55 \text{ e \AA}^{-3}$
3140 reflections	$\Delta\rho_{min} = -0.22 \text{ e \AA}^{-3}$
155 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (Å, °).

Zn1—O1	1.941 (2)	Zn1—Cl2	2.2149 (7)
Zn1—N1	2.009 (2)	Zn1—Cl1	2.2330 (8)
O1—Zn1—N1	96.84 (7)	O1—Zn1—Cl1	112.27 (6)
O1—Zn1—Cl2	111.47 (6)	N1—Zn1—Cl1	108.70 (5)
N1—Zn1—Cl2	111.01 (5)	Cl2—Zn1—Cl1	115.04 (3)

Table 2

Hydrogen-bond 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>
N2—H2B···O1 ⁱ	0.90	1.92	2.784 (2)	161
N2—H2A···Cl1	0.90	2.89	3.4401 (19)	121
N2—H2A···Cl2 ⁱⁱ	0.90	2.64	3.3749 (19)	140
C3—H3···Cl2 ⁱⁱⁱ	0.93	2.78	3.561 (2)	142

Symmetry codes: (i) *x* − 1, *y*, *z*; (ii) −*x* + $\frac{1}{2}$, *y* + $\frac{1}{2}$, −*z* + $\frac{1}{2}$; (iii) −*x* + $\frac{3}{2}$, *y* + $\frac{1}{2}$, −*z* + $\frac{1}{2}$.

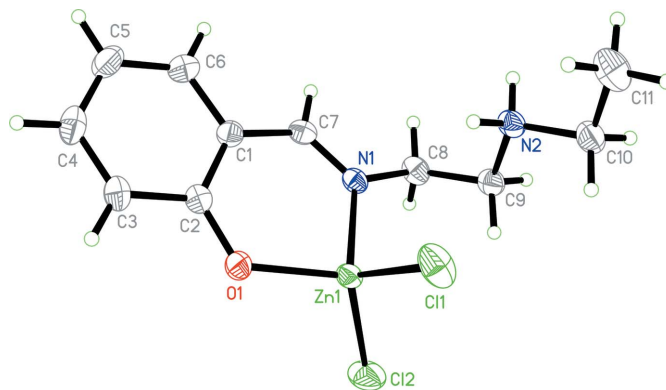


Figure 1

The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level. H atoms are represented by spheres of arbitrary radius.

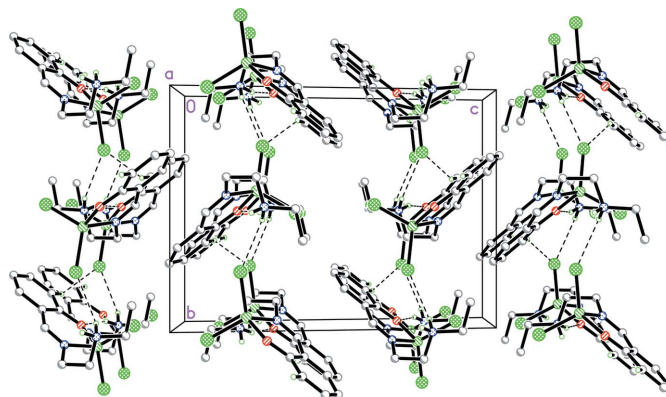


Figure 2

The crystal packing of (I). Intermolecular hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonds are omitted for clarity.

All H atoms were positioned geometrically and refined as riding, with C—H distances of 0.93–0.97 Å, N—H distances of 0.90 Å, and *U_{iso}*(H) values set at 1.2 or 1.5*U_{eq}*(C,N).

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*.

We acknowledge the Changsha University of Science and Technology for research grants.

References

- Bertini, I., Gray, H. B., Lippard, S. J. & Valentine, J. S. (1994). *Bioinorganic Chemistry*. Mills Valley, CA, USA: University Science Books.
- Bruker (2000). *SMART* (Version 5.625), *SAINT* (Version 6.01), *SHELXTL* (Version 6.10) and *SADABS* (Version 2.03). Bruker AXS Inc., Madison, Wisconsin, USA.
- Harrison, W. T. A., Ramadevi, P. & Kumaresan, S. (2006). *Acta Cryst.* **E62**, m513–m515.
- Lipscomb, W. N. & Sträter, N. (1996). *Chem. Rev.* **96**, 2375–2434.
- Musie, G. T., Li, X. & Powell, D. R. (2004). *Acta Cryst.* **E60**, m471–m472.
- Myers, L. C., Terranova, M. P., Frentz, A. E., Wagner, G. & Verdine, G. L. (1993). *Science*, **261**, 1164–1167.
- Peng, S.-J., Yang, D.-W., Xiao, Z.-L., Wu, D.-X. & Cao, Z. (2005). *Z. Kristallogr. New Cryst. Struct.* **220**, 633–634.

- Peng, S.-J., Yang, T. & Zhou, C.-S. (2006). *Acta Cryst.* **E62**, m235–m236.
- Qiu, X.-Y. (2006). *Acta Cryst.* **E62**, m717–m718.
- Tatar, L., Atakol, O. & Arici, C. (2002). *Acta Cryst.* **E58**, m154–m156.
- Tatar, L., Atakol, O. & Ülkü, D. (2002). *Acta Cryst.* **E58**, m83–m85.
- Tirosh, E., Maman, R. & Goldberg, I. (2005). *Acta Cryst.* **E61**, m751–m754.
- Ülkü, D., Arici, C., Tahir, M. N. & Atakol, O. (2000). *Acta Cryst.* **C56**, 1298–1299.
- Vallee, B. L. & Auld, D. S. (1993). *Acc. Chem. Res.* **26**, 543–551.
- Wilker, J. J. & Lippard, S. J. (1997). *Inorg. Chem.* **36**, 969–978.
- You, Z.-L. (2006). *Acta Cryst.* **E62**, m10–m11.
- You, Z.-L., Wang, J. & Han, X. (2006). *Acta Cryst.* **E62**, m714–m716.