

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

## Xiao-Yang Qiu

Department of Chemistry, Fuyang Normal College, Fuyang Anhui 236041, People's Republic of China, and Department of Chemistry and Chemical Engineering, Lanzhou University, Lanzhou 730000, People's Republic of China

Correspondence e-mail:  
xiaoyang\_qiu@126.com

## Key indicators

Single-crystal X-ray study  
T = 298 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.007 \text{ \AA}$   
R factor = 0.059  
wR factor = 0.138  
Data-to-parameter ratio = 19.6

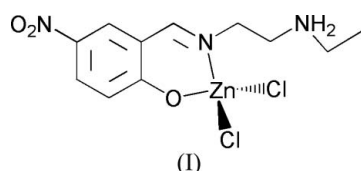
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title compound,  $[\text{ZnCl}_2(\text{C}_{11}\text{H}_{15}\text{N}_3\text{O}_3)]$ , is a mononuclear Schiff base zinc(II) complex. The Zn atom is tetrahedrally coordinated by a phenolate O atom and an imine N atom of the Schiff base, and by two chloride anions. In the crystal structure, molecules are linked through intermolecular N—H $\cdots$ O, N—H $\cdots$ Cl, C—H $\cdots$ O and C—H $\cdots$ Cl interactions, forming a three-dimensional network.

Received 7 August 2006  
Accepted 9 August 2006

## Comment

Zinc(II) complexes are very important in biological chemistry (Weston, 2005; Henkel & Krebs, 2004). They function as the active site of hydrolytic enzymes, such as carboxypeptidase and carbonic anhydrase (Bertini *et al.*, 1994; Lipscomb & Sträter, 1996). The structure of a new zinc(II) complex, (I), derived from the Schiff base 4-nitro-2-[2-(ethylamino)ethyliminomethyl]phenol is reported here.



Compound (I) is a mononuclear zinc(II) complex, in which the Schiff base ligand is in a zwitterionic form, with the ethylamino N atom protonated (Fig. 1). The Zn atom is tetrahedrally coordinated by the phenolate O atom and the imine N atom of the Schiff base, and by two chloride anions. The Zn—O and Zn—N bond lengths (Table 1) are comparable with the corresponding values observed in other Schiff base zinc(II) complexes (Tatar *et al.*, 1999; Qiu, 2006). Atoms in the N1/C8/C9/N3/C10/C11 chain adopt a *trans* configuration to minimize steric effects.

In the crystal structure, molecules are linked through intermolecular N—H $\cdots$ O, N—H $\cdots$ Cl, C—H $\cdots$ O and C—H $\cdots$ Cl interactions (Table 2), forming a three-dimensional network.

## Experimental

A mixture of 5-nitrosalicylaldehyde (1.0 mmol, 167.3 mg), *N*-ethyl-1,2-diaminoethane (1.0 mmol, 88.1 mg) and  $\text{ZnCl}_2$  (1.0 mmol, 136.3 mg) was dissolved in ethanol (100 ml). The mixture was stirred for about 1 h at room temperature to give a clear colourless solution. After allowing the solution to stand still in air for 5 d, colourless block-shaped crystals formed.

Crystal data

[ZnCl<sub>2</sub>(C<sub>11</sub>H<sub>15</sub>N<sub>3</sub>O<sub>3</sub>)]

*M<sub>r</sub>* = 373.53

Monoclinic, *P*2<sub>1</sub>/*c*

*a* = 11.879 (2) Å

*b* = 11.478 (2) Å

*c* = 12.612 (2) Å

β = 115.077 (3)°

*V* = 1557.5 (5) Å<sup>3</sup>

*Z* = 4

*D<sub>x</sub>* = 1.593 Mg m<sup>-3</sup>

Mo *K*α radiation

μ = 1.93 mm<sup>-1</sup>

*T* = 298 (2) K

Block, colourless

0.12 × 0.10 × 0.07 mm

Data collection

Bruker SMART APEX 1000 CCD

area-detector diffractometer

ω scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

*T<sub>min</sub>* = 0.802, *T<sub>max</sub>* = 0.877

13152 measured reflections

3559 independent reflections

2082 reflections with *I* > 2σ(*I*)

*R<sub>int</sub>* = 0.094

θ<sub>max</sub> = 27.5°

Refinement

Refinement on *F*<sup>2</sup>

*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.059

*wR* (*F*<sup>2</sup>) = 0.138

*S* = 1.02

3559 reflections

182 parameters

H-atom parameters constrained

*w* = 1/[σ<sup>2</sup>(*F<sub>o</sub>*<sup>2</sup>) + (0.0366*P*)<sup>2</sup>]

where *P* = (*F<sub>o</sub>*<sup>2</sup> + 2*F<sub>c</sub>*<sup>2</sup>)/3

(Δ/σ)<sub>max</sub> < 0.001

Δρ<sub>max</sub> = 0.43 e Å<sup>-3</sup>

Δρ<sub>min</sub> = -0.40 e Å<sup>-3</sup>

Table 1

Selected geometric parameters (Å, °).

Zn1—O1	1.958 (3)	Zn1—Cl2	2.2074 (14)
Zn1—N2	1.999 (4)	Zn1—Cl1	2.2487 (15)
O1—Zn1—N2	96.85 (14)	O1—Zn1—Cl1	110.23 (11)
O1—Zn1—Cl2	106.81 (10)	N2—Zn1—Cl1	109.90 (11)
N2—Zn1—Cl2	112.60 (11)	Cl2—Zn1—Cl1	118.26 (5)

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>
N3—H3B...O1 <sup>i</sup>	0.90	1.97	2.857 (5)	167
N3—H3A...Cl1	0.90	2.71	3.350 (4)	129
N3—H3A...Cl2 <sup>l</sup>	0.90	2.61	3.300 (4)	134
C7—H7...Cl1 <sup>l</sup>	0.93	2.74	3.583 (4)	151
C9—H9A...Cl1 <sup>ii</sup>	0.97	2.78	3.684 (4)	156
C10—H10B...O3 <sup>iii</sup>	0.97	2.39	3.261 (4)	149

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

H atoms were placed in calculated positions and constrained to ride on their parent atoms, with N—H = 0.90 Å, C—H = 0.93–0.97 Å and *U*<sub>iso</sub>(H) = 1.2 or 1.5*U*<sub>eq</sub>(C,N).

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*.

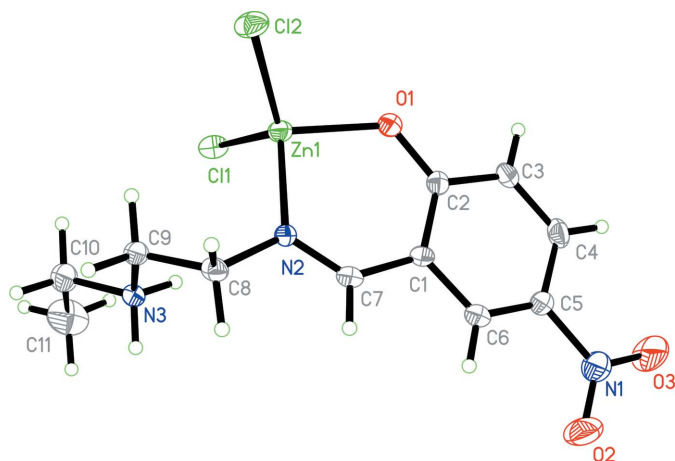


Figure 1

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

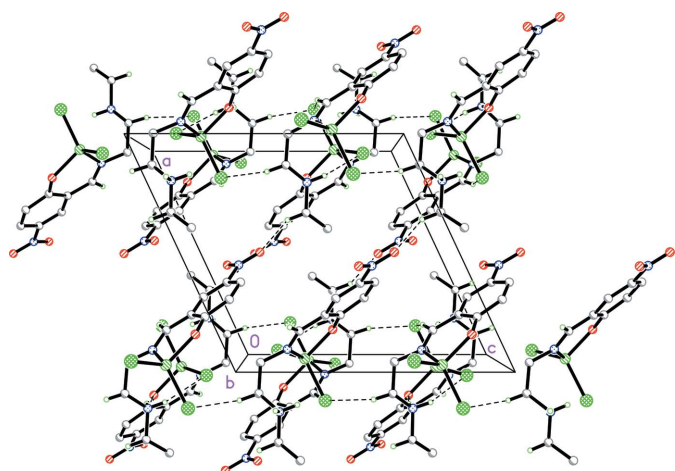


Figure 2

The crystal packing of (I). Intermolecular N—H...O, N—H...Cl, C—H...O, and C—H...Cl hydrogen bonds are shown as dashed lines.

The author acknowledges a research grant from Fuyang Normal College.

References

- Bertini, I., Gray, H. B., Lippard, S. J. & Valentine, J. S. (1994). *Bioinorganic Chemistry*. Mills Valley, CA: University Science Books.
- Bruker (1998). *SMART* (Version 5.628) and *SAINT* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
- Henkel, G. & Krebs, B. (2004). *Chem. Rev.* **104**, 801–824.
- Lipscomb, W. N. & Sträter, N. (1996). *Chem. Rev.* **96**, 2375–2434.
- Qiu, X.-Y. (2006). *Acta Cryst.* **E62**, m717–m718.
- Sheldrick, G. M. (1996). *SADABS*. Version 2.03. 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.
- Tatar, L., Ülkü, D. & Atakol, O. (1999). *Acta Cryst.* **C55**, 508–510.
- Weston, J. (2005). *Chem. Rev.* **105**, 2151–2174.