Zhong-Lu You

Department of Chemistry and Chemical Engineering, Liaoning Normal University, Dalian 116029, People's Republic of China

Correspondence e-mail: youzhonglu@yahoo.com.cn

Key indicators

Single-crystal X-ray study
$T = 298$ K
Mean σ(C–C) = 0.004 Å
R factor = 0.041
wR factor = 0.105
Data-to-parameter ratio = 18.5

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

In the mononuclear title complex, $[Zn(C_{10}H_8Cl_2NO)_2]$,the Zn^{II} atom is four-coordinated in a distorted tetrahedral configuration by two imine N and two phenolate O atoms from two Schiff base ligands.

Comment

Recently, the crystal structures of some Schiff base zinc(II) compounds have been reported (You, 2005a,b,c). In continuation of the work on these compounds, the title zinc(II) compound, (I), is reported here.

(I)
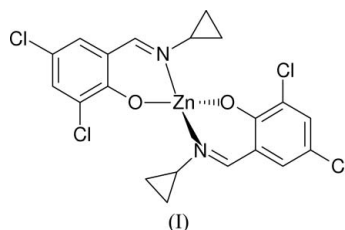
Complex (I) is a mononuclear zinc(II) compound (Fig. 1), which is structurally similar to bis[2-(cyclopropyliminomethyl)phenolato]zinc(II) [(II); You *et al.*, 2003]. The bond lengths and angles (Table 1) are comparable to those in (II). As observed in (II), the central Zn^{II} atom is four-coordinated by two imine N and two phenolate O atoms from two Schiff base ligands. The angles subtended at the Zn^{II} atom [range 95.73 (8)–120.78 (9)°] indicate a distorted tetrahedral geometry. In the crystal packing, symmetry-related molecules are linked *via* C—H···Cl hydrogen bonds (Table 2) into a three-dimensional framework.

Experimental

Cyclopropylamine (0.1 mmol, 5.7 mg) and 3,5-dichloro-salicylaldehyde (0.1 mmol, 19.2 mg) were dissolved in MeOH (10 ml). The mixture was stirred at room temperature for 10 min to give a clear yellow solution. To this solution was added a MeOH solution (5 ml) of $Zn(CH_3COO)_2 \cdot 4H_2O$ (0.1 mmol, 25.6 mg), with stirring. The resulting mixture was stirred for another 10 min at room temperature. After keeping the filtrate in air for 5 d, colourless plate-shaped crystals were formed at the bottom of the vessel.

Crystal data

$[Zn(C_{10}H_8Cl_2NO)_2]$	$D_x = 1.642$ Mg m^{-3}
$M_r = 523.52$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 4332
$a = 23.574$ (2) Å	reflections
$b = 7.926$ (1) Å	$\theta = 2.7$–24.2°
$c = 24.264$ (2) Å	$\mu = 1.68$ mm^{-1}
$\beta = 110.881$ (1)°	$T = 298$ (2) K
$V = 4235.9$ (7) Å^3	Plate, colourless
$Z = 8$	$0.22 \times 0.18 \times 0.09$ mm

Data collection

Bruker SMART CCD area-detector diffractometer	4834 independent reflections
	3757 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.035$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$\theta_{max} = 27.5°$
	$h = -30 \rightarrow 30$
$T_{min} = 0.708$, $T_{max} = 0.863$	$k = -10 \rightarrow 10$
17686 measured reflections	$l = -31 \rightarrow 31$

Refinement

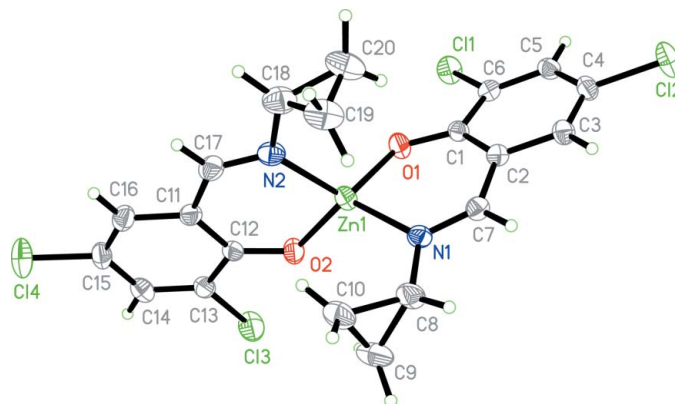|	
Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0439P)^2 + 4.452P]$
$R[F^2 > 2\sigma(F^2)] = 0.041$	
$wR(F^2) = 0.105$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.001$
4834 reflections	$\Delta\rho_{max} = 0.54$ e Å^{-3}
262 parameters	$\Delta\rho_{min} = -0.39$ e Å^{-3}
H-atom parameters constrained	

Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

Table 1
Selected geometric parameters (Å, °).

Zn1—O2	1.895 (2)	Zn1—N1	2.008 (2)
Zn1—O1	1.917 (2)	Zn1—N2	2.017 (2)
O2—Zn1—O1	112.73 (9)	O2—Zn1—N2	96.27 (9)
O2—Zn1—N1	120.78 (9)	O1—Zn1—N2	117.88 (9)
O1—Zn1—N1	95.73 (8)	N1—Zn1—N2	115.06 (9)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10A···Cl3^i	0.97	2.81	3.757 (3)	167
C17—H17···Cl1^{ii}	0.93	2.83	3.747 (3)	170

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

H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.98 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

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*.

References

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