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Bis[4-chloro-2-(cyclohexyliminomethyl)-phenolato]zinc(II)

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.004 Å
R factor = 0.037
wR factor = 0.075
Data-to-parameter ratio = 15.7

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

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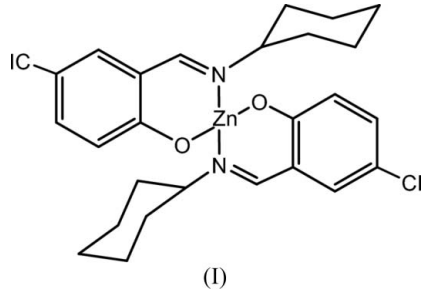
In the mononuclear title compound, $[Zn(C_{13}H_{15}ClNO)_2]$, the Zn^{II} atom is four-coordinated by two N atoms and two O atoms from two Schiff base ligands in a slightly distorted tetrahedral geometry.

Comment

Transition metal compounds containing Schiff base ligands have been of great interest for a long time. These compounds play an important role in the development of the coordination chemistry related to catalysis and enzymatic reactions, magnetism and molecular architectures (Costamagna *et al.*, 1992; Bhatia *et al.*, 1981). As an extension of work on the structural characterization of Schiff base–zinc(II) compounds, the crystal structure of the title compound, (I), is reported here.



(I)

Compound (I) is a mononuclear Zn^{II} complex (Fig. 1). It is structurally similar to the nickel(II) and cobalt(II) complexes derived from other Schiff base ligands (Steward *et al.*,1961; Erxleben & Schumacher, 2001). The Zn^{II} ion is coordinated by two O and two N atoms from two Schiff base ligands. This ZnN_2O_2 coordination forms a distorted tetrahedral geometry, with angles subtended at the Zn^{II} atom in the range 94.72 (9)–122.35 (9)° (Table 1). The bond lengths around the Zn atom range from 1.910 (2) to 2.019 (2) Å.

Experimental

5-Chlorosalicylaldehyde (0.1 mmol, 15.7 mg), $Zn(CH_3COO)_2\cdot 2H_2O$ (0.1 mmol, 22.0 mg) and cyclohexanamine (0.1 mmol, 9.3 mg) were dissolved in methanol (10 ml). The mixture was stirred for 30 min at room temperature to give a clear brown solution. After allowing the resulting solution to stand in air for 11 d, brown block-shaped crystals of (I) were formed on slow evaporation of the solvent. The crystals were collected, washed with methanol and dried in a vacuum desiccator using anhydrous $CaCl_2$ (yield 54%). Analysis found: C 57.9, H 5.56%; calculated for $C_{26}H_{30}Cl_2N_2O_2Zn$: C 58.0, H 5.57%.

Crystal data

$\{Zn(C_{13}H_{15}ClNO)_2\}$	Mo $K\alpha$ radiation
M_r = 538.79	Cell parameters from 30 reflections
Orthorhombic, *Pbca*	θ = 2.2–13.6°
a = 14.848 (2) Å	μ = 1.21 mm^{-1}
b = 13.567 (2) Å	T = 296 (2) K
c = 24.993 (5) Å	Block, brown
V = 5034.5 (13) Å^3	0.68 × 0.50 × 0.24 mm
Z = 8	
D_x = 1.422 Mg m^{-3}	

Data collection

Siemens P4 diffractometer	R_{int} = 0.024
ω scans	θ_{max} = 25.5°
Absorption correction: ψ scan (*XSCANS*; Siemens, 1995)	$h = 0 \rightarrow 17$
	$k = 0 \rightarrow 16$
T_{min} = 0.472, T_{max} = 0.747	$l = -30 \rightarrow 1$
5714 measured reflections	3 standard reflections
4687 independent reflections	every 97 reflections
2587 reflections with $I > 2\sigma(I)$	intensity decay: 3.4%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0308P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.037	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.075	$\Delta\rho_{max}$ = 0.23 e Å^{-3}
S = 0.90	$\Delta\rho_{min}$ = −0.34 e Å^{-3}
4687 reflections	Extinction correction: *SHELXL97*
299 parameters	Extinction coefficient: 0.00191 (12)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Zn—O2	1.910 (2)	Zn—N2	2.015 (2)
Zn—O1	1.922 (2)	Zn—N1	2.019 (2)
O2—Zn—O1	120.24 (9)	O2—Zn—N1	113.23 (9)
O2—Zn—N2	95.61 (9)	O1—Zn—N1	94.72 (9)
O1—Zn—N2	112.72 (9)	N2—Zn—N1	122.35 (9)

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

Data collection: *XSCANS* (Siemens, 1995); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Siemens, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXL97*.

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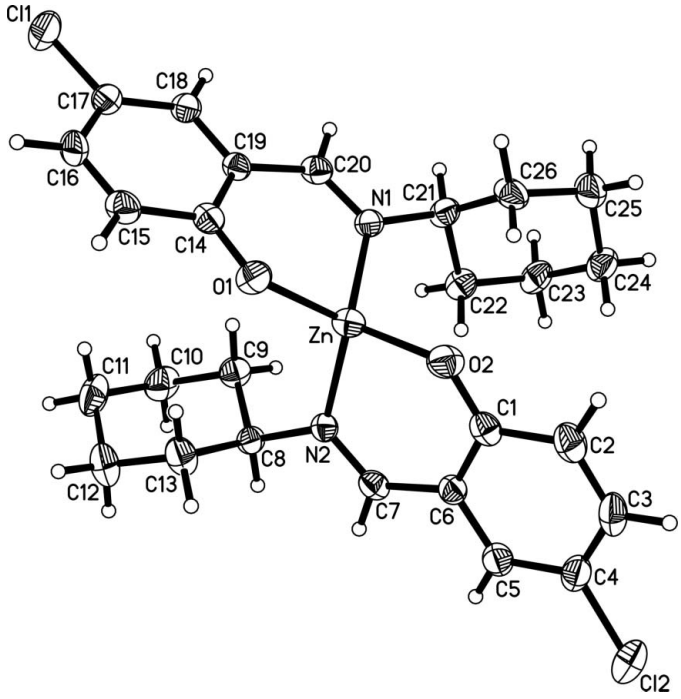

Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

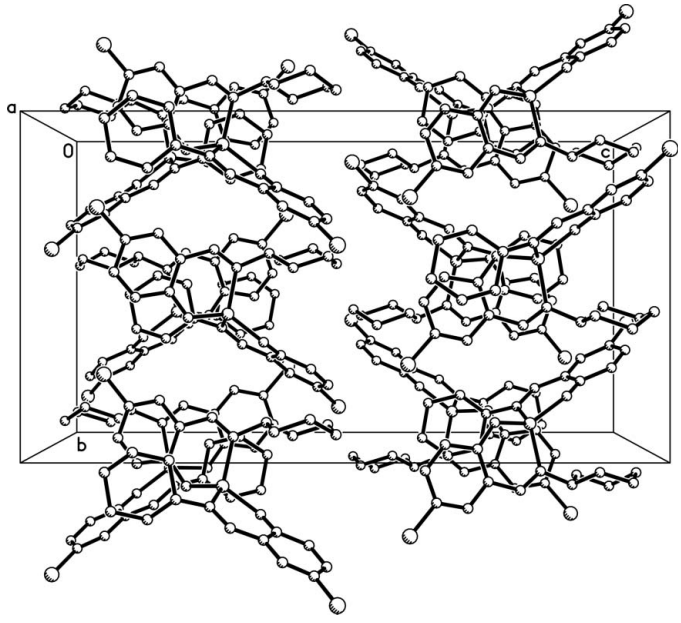

Figure 2
The crystal packing of (I), viewed along the *a* axis. H atoms have been omitted.

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