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Dichloro{2-[3-(cyclohexylammonio)propyliminomethyl]-6-methylphenolato}zinc(II)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
Disorder in main residue
R factor = 0.040
wR factor = 0.115
Data-to-parameter ratio = 17.0

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

In the mononuclear title compound, $[ZnCl_2(C_{17}H_{26}N_2O)]$, the Zn^{II} atom is four-coordinated in a tetrahedral configuration by one imine N and one phenolate O atoms from a Schiff base ligand, and by two terminal Cl atoms. In the crystal structure, the molecules are linked through intermolecular N—H···Cl hydrogen bonds, forming chains running along the b axis.

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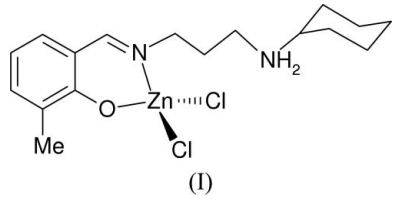
Comment

The crystal structures of a few Schiff base zinc(II) compounds have already been reported from this laboratory (You, 2005*a*,*b*,*c*). As an extension 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). The Zn^{II} atom is four-coordinated by one imine N and one phenolate O atoms from a Schiff base ligand, and by two terminal Cl atoms, forming a tetrahedral coordination. The Zn—N and Zn—O bond lengths and angles (Table 1) subtended at the Zn1 atom are comparable to the values observed in the Schiff base zinc(II) complexes cited above. As expected, the cyclohexyl group adopts a chair conformation to minimize steric effects.

In the crystal structure, molecules are linked through intermolecular N—H···Cl hydrogen bonds, forming chains running along the b axis (Fig. 2 and Table 2).

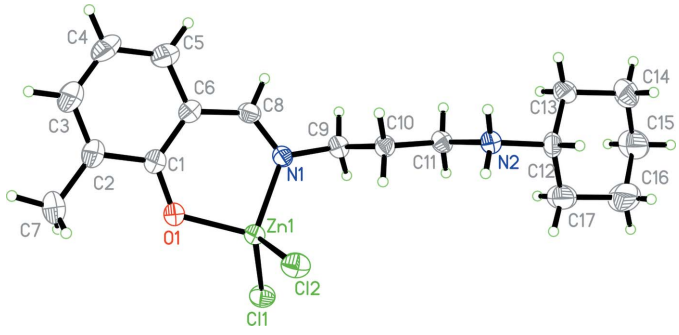


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Only the major component of the disordered cyclohexyl group is shown.

Experimental

N-Cyclohexyl-1,3-diaminopropane (0.1 mmol, 15.6 mg) and 3-methylsalicylaldehyde (0.1 mmol, 13.6 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 an MeOH solution (5 ml) of $ZnCl_2$ (0.1 mmol, 13.6 mg), with stirring. The resulting mixture was stirred for another 10 min at room temperature. After keeping the filtrate in air for 16 d, colourless block-shaped crystals were formed at the bottom of the vessel.

Crystal data

$[ZnCl_2(C_{17}H_{26}N_2O)]$	D_x = 1.449 Mg m^{-3}
M_r = 410.67	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 5157 reflections
a = 35.492 (3) Å	θ = 2.7–25.0°
b = 7.482 (1) Å	μ = 1.59 mm^{-1}
c = 15.011 (1) Å	T = 298 (2) K
β = 109.132 (1)°	Block, colourless
V = 3766.0 (6) Å^3	0.25 × 0.24 × 0.13 mm
Z = 8	

Data collection

Bruker SMART CCD area-detector diffractometer	4483 independent reflections
	3472 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.026
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	θ_{max} = 28.4°
	$h = -46 \rightarrow 45$
T_{min} = 0.692, T_{max} = 0.820	$k = -9 \rightarrow 9$
15865 measured reflections	$l = -19 \rightarrow 19$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.065P)^2 + 2.2034P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.040	
$wR(F^2)$ = 0.115	
S = 1.04	$(\Delta/\sigma)_{max}$ = 0.001
4483 reflections	$\Delta\rho_{max}$ = 0.56 e Å^{-3}
264 parameters	$\Delta\rho_{min}$ = −0.29 e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.915 (2)	Zn1—Cl1	2.2373 (8)
Zn1—N1	2.007 (2)	Zn1—Cl2	2.2606 (8)
O1—Zn1—N1	96.43 (9)	O1—Zn1—Cl2	111.78 (8)
O1—Zn1—Cl1	108.55 (8)	N1—Zn1—Cl2	109.86 (6)
N1—Zn1—Cl1	114.37 (7)	Cl1—Zn1—Cl2	114.46 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···Cl1^{i}	0.90	2.35	3.254 (3)	177
N2—H2B···Cl2^{ii}	0.90	2.44	3.325 (2)	167

Symmetry codes: (i) $-x+\frac{3}{2}, -y+\frac{5}{2}, -z+2$; (ii) $-x+\frac{3}{2}, -y+\frac{3}{2}, -z+2$.

The cyclohexyl group is disordered over two sites, with occupancy factors of 0.761 (6) and 0.239 (6). The C—C and N—C distances involving the disordered atoms were restrained to 1.53 (1) and 1.46 (1) Å, respectively. The U^{ij} components of the disordered atoms were approximated to isotropic behaviour. 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, N—H distances of 0.90 Å, and with U_{iso}(H) = 1.2–1.5U_{eq}(C,N).

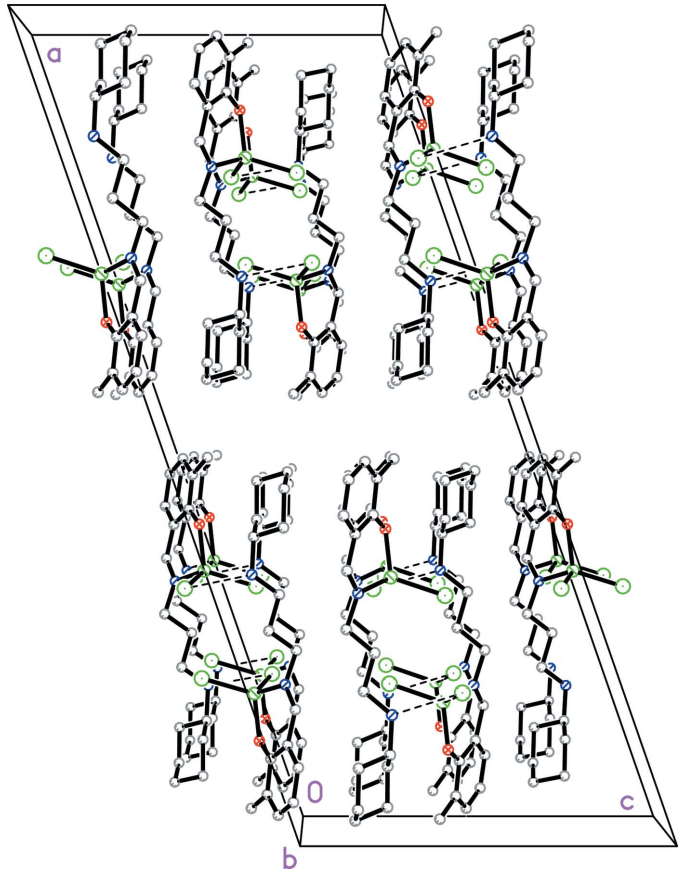


Figure 2
The crystal packing of (I), viewed along the *b* axis. Intermolecular hydrogen bonds are shown as dashed lines. H atoms have been omitted for clarity.

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*.

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