Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Dichloro[*N*,*N*-dimethyl-*N*′-(pyridin-2-ylmethylidene)-ethane-1,2-diamine]zinc(II)

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.031
wR factor = 0.070
Data-to-parameter ratio = 20.2

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

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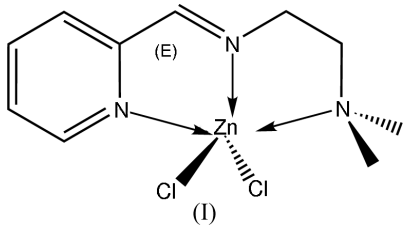
Received 19 January 2005
Accepted 21 January 2005
Online 29 January 2005

The title compound, $[ZnCl_2(C_{10}H_{15}N_3)]$, is a mononuclear zinc(II) complex in which the Zn^{II} atom is five-coordinated by three N atoms of the Schiff base ligand, and two Cl^- anions, forming a distorted square-pyramidal coordination geometry.

Comment

Transition metal compounds are present in the active sites of several important classes of metalloproteins. The study of Schiff base compounds is of great interest in various areas of chemistry (Downing & Urbach, 1969; Ganeshpure *et al.*, 1996; Bosnich, 1968; Costes *et al.*, 1995). As an extension of our work on the structural characterization of Schiff base complexes, the mononuclear Schiff base zinc(II) complex, (I), is described here.



(I)

Complex (I) is a mononuclear zinc(II) compound (Fig. 1). Selected bond distances and angles are given in Table 1. Atom Zn1 has a square-pyramidal coordination geometry involving three N atoms from the Schiff base ligand *N*,*N*-dimethyl-*N*′-(pyridin-2-ylmethylidene)ethane-1,2-diamine and atom Cl2 in the basal plane, with atom Cl1 in the apical position. A significant distortion of the square pyramid is revealed by the angles between the apical and basal donor atoms (Table 1), which show an average deviation of 16.32° from the ideal 90° angle found in a regular square pyramid. The angles for the basal donor atoms [74.21 (8)° for N2—Zn1—N1 and 76.82 (7)° for N2—Zn1—N3] correlate with the strained ligand bite angles for the five-membered chelate rings Zn1—N1—C5—C6—N2 and Zn1—N2—C7—C8—N3, respectively. The other basal angles are closer to 90° [range 98.27 (5)–114.03 (3)°]. The value of the N2═C6 bond length in (I) is 1.258 (3) Å, which conforms to the value for a double bond, while the N2—C7 bond length is 1.460 (3) Å, which conforms to the value for a C—N single bond.

In the crystal structure, the molecules stack along the *a* axis with no short contacts (Fig. 2).

Experimental

2–Pyridylaldehyde (0.1 mmol, 10.7 mg) and *N*,*N*-dimethylethane-1,2-diamine (0.1 mmol, 8.8 mg) were dissolved in ethanol (10 ml). The

mixture was stirred for 15 min to give a clear yellow solution. To this solution was added an ethanol solution (5 ml) of $ZnCl_2·4H_2O$ (0.1 mmol, 17.3 mg), with stirring. The mixture was stirred at room temperature for about 30 min and then filtered. After allowing the colorless filtrate to stand in air for 7 d, colorless block-shaped crystals were formed at the bottom of the vessel on slow evaporation of the solvent.

Crystal data

$[ZnCl_2(C_{10}H_{15}N_3)]$	$Z = 2$
$M_r = 313.52$	$D_x = 1.589$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 7.298$ (1) Å	Cell parameters from 3473 reflections
$b = 8.003$ (1) Å	$\theta = 2.7$–$27.1°$
$c = 11.985$ (2) Å	$\mu = 2.26$ mm^{-1}
$\alpha = 100.18$ (1)°	$T = 295$ (2) K
$\beta = 101.95$ (1)°	Block, colorless
$\gamma = 100.86$ (1)°	0.21 × 0.07 × 0.07 mm
$V = 655.4$ (2) Å^3	

Data collection

Bruker SMART APEX area-detector diffractometer	2965 independent reflections
ω scans	2681 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.023$
$T_{min} = 0.649$, $T_{max} = 0.858$	$\theta_{max} = 27.5°$
7557 measured reflections	$h = -9 \rightarrow 9$
	$k = -10 \rightarrow 10$
	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0288P)^2 + 0.1151P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.031$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.070$	$\Delta\rho_{max} = 0.34$ e Å^{-3}
$S = 1.09$	$\Delta\rho_{min} = -0.24$ e Å^{-3}
2965 reflections	
147 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Zn1—N2	2.106 (2)	Zn1—N3	2.271 (2)
Zn1—N1	2.236 (2)	N2—C6	1.258 (3)
Zn1—Cl2	2.255 (1)	N2—C7	1.460 (3)
Zn1—Cl1	2.255 (1)		
N2—Zn1—N1	74.21 (8)	Cl2—Zn1—Cl1	114.03 (3)
N2—Zn1—Cl2	132.12 (6)	N2—Zn1—N3	76.82 (7)
N1—Zn1—Cl2	95.87 (5)	N1—Zn1—N3	150.29 (7)
N2—Zn1—Cl1	113.73 (6)	Cl2—Zn1—N3	98.64 (5)
N1—Zn1—Cl1	98.27 (5)	Cl1—Zn1—N3	99.26 (5)

The H atoms were positioned geometrically and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å and with $U_{iso}(H) = 1.2$ or $1.5U_{eq}(C)$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXTL*.

The author thanks Qufu Normal University for funding this study.

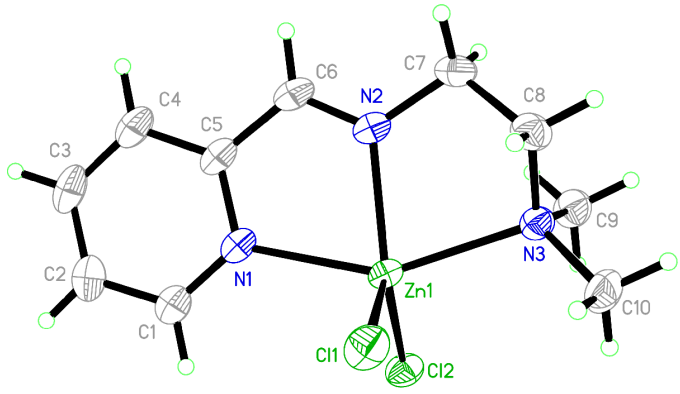


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

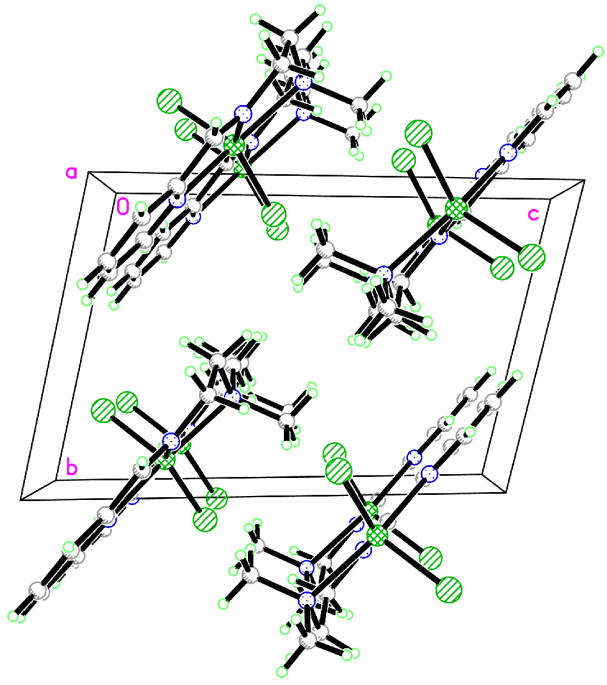


Figure 2
The crystal packing of (I), viewed along the *a* axis.

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