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Dichlorobis(1-methylimidazole)zinc(II)

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.003 Å
R factor = 0.022
wR factor = 0.059
Data-to-parameter ratio = 17.7

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

The zinc(II) ion in the title compound, $[ZnCl_2(C_4H_6N_2)_2]$, has a distorted tetrahedral geometry with a Cl_2N_2 environment.

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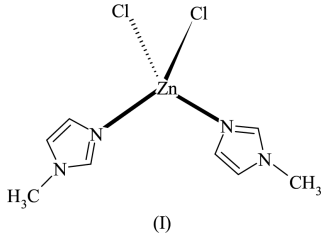
Comment

The zinc(II) ion is a biologically and pharmaceutically essential component. The synthesis and characterization of zinc complexes with biologically relevant ligands has been a subject of interest for many years (Dakternieks, 1990, and references therein). Whereas some work has been reported on the synthesis and characterization of imidazole–zinc(II) complexes, fewer complexes have been reported with 1-methylimidazole (Tolman *et al.*, 1991; Bharadwaj *et al.*, 1991). As part of a general method for the preparation of biologically relevant zinc(II) complexes, we prepared the title compound, (I).



(I)

The molecular structure and packing diagram of (I) are shown in Figs. 1 and 2, respectively. The zinc(II) center of the complex is coordinated by two 1-methylimidazole molecules and two chloride ligands in a slightly distorted tetrahedral geometry. The Zn—Cl and Zn—N bond distances are similar to those in other zinc complexes reported in the literature. Deviation from regular tetrahedral geometry is shown particularly by the large Cl1—Zn1—Cl2 angle of 118.19 (17)°.

Experimental

A methanol solution (10 ml) of $ZnCl_2$ (0.73 g, 10 mmol) was added to a methanol solution (10 ml) of 1-methylimidazole (1.64 g, 20 mmol). After stirring the reaction mixture for 4 h at room temperature, the solution was concentrated by partial removal of the solvent *in vacuo*. Slow ether diffusion into the concentrated solution yielded colorless block-shaped crystals of (I).

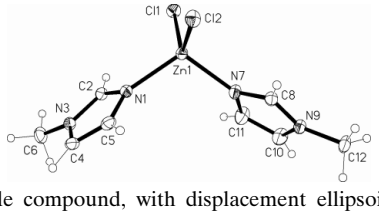


Figure 1
View of the title compound, with displacement ellipsoids at the 50% probability level.

Crystal data

$[ZnCl_2(C_4H_6N_2)_2]$	D_x = 1.620 Mg m^{-3}
M_r = 300.49	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 8529 reflections
a = 7.946 (3) Å	θ = 2.3–26.0°
b = 12.385 (4) Å	μ = 2.40 mm^{-1}
c = 12.741 (4) Å	T = 100 (2) K
β = 100.789 (5)°	Block, colorless
V = 1231.7 (7) Å^3	0.50 × 0.48 × 0.24 mm
Z = 4	

Data collection

Bruker SMART APEX diffractometer	2410 independent reflections
	2289 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.033
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)	θ_{max} = 26.0°
	$h = -9 \rightarrow 9$
T_{min} = 0.314, T_{max} = 0.560	$k = -15 \rightarrow 15$
10426 measured reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.033P)^2 + 0.55P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.022	
$wR(F^2)$ = 0.059	
S = 1.02	$(\Delta/\sigma)_{max}$ = 0.002
2410 reflections	$\Delta\rho_{max}$ = 0.30 e Å^{-3}
136 parameters	$\Delta\rho_{min}$ = −0.29 e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Zn1—N7	2.0055 (14)	Zn1—Cl2	2.2460 (7)
Zn1—N1	2.0081 (14)	Zn1—Cl1	2.2495 (9)
N7—Zn1—N1	109.60 (6)	N7—Zn1—Cl1	108.29 (4)
N7—Zn1—Cl2	106.10 (5)	N1—Zn1—Cl1	103.48 (5)
N1—Zn1—Cl2	111.02 (4)	Cl2—Zn1—Cl1	118.199 (17)

H atoms were positioned geometrically (C—H = 0.95–0.98 Å) and treated as riding. H-atom displacement parameters were set at 1.2 (1.5 for methyl) times U_{eq} of the bonded atoms.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

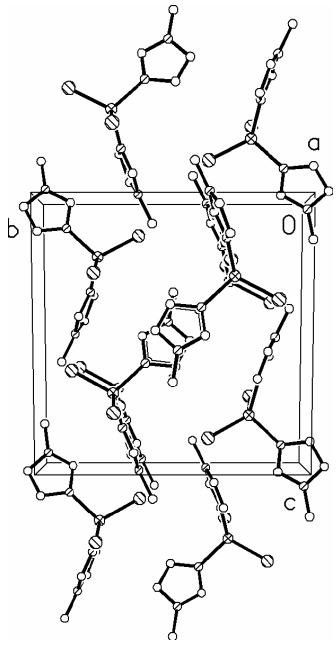


Figure 2
Packing diagram of the title compound displaying the unit cell, viewed down the *c* axis. H atoms have been omitted for clarity.

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