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Dichlorobis(2-methoxymethyl-1-methyl-1*H*-imidazole-κN)zinc(II)

Hong-Mei Chen, Jing-Jia Sun, Jia-Min Chen and Shi-Ping Yang*

School of Chemistry, Shanghai Teacher University, Shanghai 200234, People's Republic of China

Correspondence e-mail: shipingy@shnu.edu.cn

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.051
wR factor = 0.133
Data-to-parameter ratio = 18.6

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

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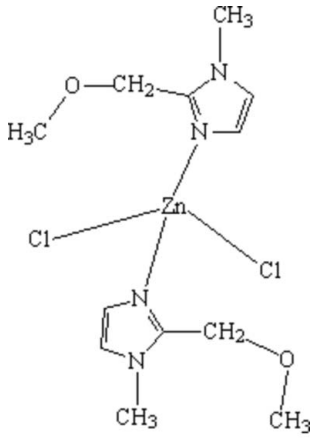
In the title Zn^{II} complex, $[ZnCl_2(C_6H_{10}N_2O)_2]$, the Zn atom is coordinated by two Cl atoms and two imidazole N atoms in a distorted tetrahedral geometry. Weak intermolecular C—H···O hydrogen bonding occurs between the methyl and methoxy groups.

Comment

As a part of our ongoing studies on metal complexes incorporating imidazole and related ligands (Yang *et al.*, 1999; Yang, Chen, Zhang, Chen & Yu, 2004; Yang, Chen, Zhang & Yu, 2004), we present here the structure of the title complex, (I).



(I)

The Zn atom is coordinated by two Cl and two imidazole N atoms in a distorted tetrahedral coordination environment (Fig. 1 and Table 1). Imidazole rings in the same complex are nearly perpendicular to each other, the dihedral angle being 81.1 (4)°. The organic ligands of methylmethoxymethylimidazole show different conformations, the methoxy groups being extended along different directions with respect to the imidazole rings. The C3—C4—O1—C5 and C9—C10—O2—C11 torsion angles are 162.9 (4) and 66.4 (4)°, respectively.

Weak intermolecular C—H···O hydrogen bonding occurs between the methyl and methoxy groups (Table 2).

Experimental

An ethanol solution (10 ml) of methylmethoxymethylimidazole (2 mmol, 0.25 g) was mixed with a methanol solution (20 ml) of $ZnCl_2{\cdot}6H_2O$ (1 mmol, 0.24 g). The mixture was stirred for 1 h at room temperature and then filtered. Crystals of (I) were obtained from the filtrate after 5 d.

Crystal data

$[ZnCl_2(C_6H_{10}N_2O)_2]$	$Z = 2$
$M_r = 388.59$	$D_x = 1.518$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 7.2084$ (7) Å	Cell parameters from 2869 reflections
$b = 8.9384$ (8) Å	$\theta = 2.3$–$27.0°$
$c = 13.4894$ (12) Å	$\mu = 1.77$ mm^{-1}
$\alpha = 95.718$ (2)°	$T = 298$ (2) K
$\beta = 94.078$ (2)°	Block, colorless
$\gamma = 99.206$ (2)°	0.52 × 0.50 × 0.21 mm
$V = 850.32$ (14) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	3607 independent reflections
φ and ω scans	3148 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)	$R_{int} = 0.086$
$T_{min} = 0.429$, $T_{max} = 0.670$	$\theta_{max} = 27.0°$
5036 measured reflections	$h = -9 \rightarrow 9$
	$k = -11 \rightarrow 9$
	$l = -14 \rightarrow 17$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.051$	$w = 1/[\sigma^2(F_o^2) + (0.0833P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.133$	$(\Delta/\sigma)_{max} = 0.002$
$S = 1.04$	$\Delta\rho_{max} = 0.81$ e Å^{-3}
3607 reflections	$\Delta\rho_{min} = -1.17$ e Å^{-3}
194 parameters	

Table 1
Selected geometric parameters (Å, °).

Zn—N1	2.026 (2)	Zn—Cl1	2.2445 (8)
Zn—N3	2.011 (2)	Zn—Cl2	2.2204 (9)
N3—Zn—N1	107.25 (10)	N3—Zn—Cl1	107.24 (7)
N3—Zn—Cl2	111.34 (7)	N1—Zn—Cl1	106.96 (7)
N1—Zn—Cl2	107.49 (8)	Cl2—Zn—Cl1	116.15 (4)

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6*C*···O1^{i}	0.96	2.32	3.276 (5)	177

Symmetry code: (i) $-x, -y+1, -z+1$.

Methyl H atoms were placed in calculated positions, with C—H = 0.96 Å, and their torsion angles were refined to fit the electron density, with U_{iso}(H) = 1.5U_{eq}(C). Other H were positioned geometrically, with C—H = 0.93 (aromatic) or 0.97 Å(methylene) and refined using the riding-model approximation, with 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); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

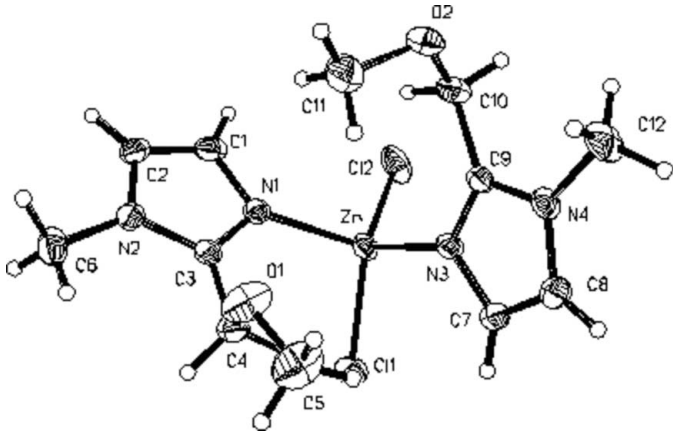


Figure 1
The structure of (I), with 30% probability displacement ellipsoids.

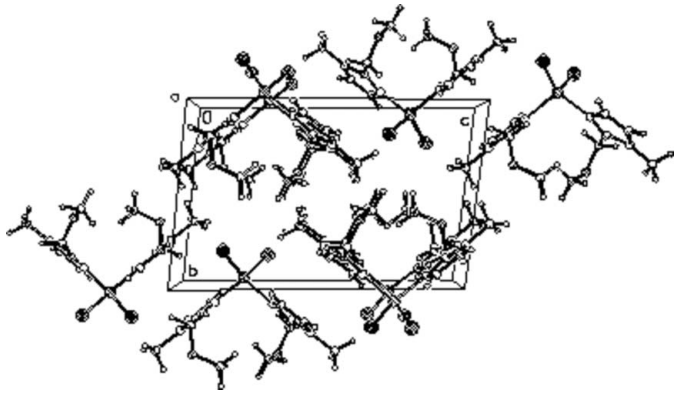


Figure 2
Perspective view of the packing of the title compound, viewed down the *a* axis

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