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cis-Dichlorobis[2-(2-pyridyl)-1*H*-imidazole-κN^3]zinc(II) hemihydrate

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Key indicators

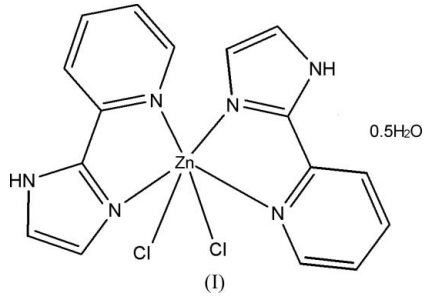
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
Disorder in solvent or counterion
R factor = 0.028
wR factor = 0.091
Data-to-parameter ratio = 17.1

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

In the title mononuclear zinc complex, $[ZnCl_2(C_8H_7N_3)_2]\cdot 0.5H_2O$, the Zn atom is located on a twofold axis and has a slightly distorted octahedral geometry consisting of four N atoms from two 2-(2-pyridyl)imidazole ligands and two Cl^- anions. The complex molecules are connected through intermolecular hydrogen bonds, forming a two-dimensional layer structure.

Comment

In recent years, much of the work on coordination polymers has been focused on metal complexes with bidentate chelating ligands because of their fascinating structural diversity and the potential applications as functional materials of these polymers (Zhang *et al.*, 2003; Lan *et al.*, 2006). Weak interactions, such as hydrogen bonding and π–π stacking, have attracted interest for their significance in chemistry and biology, especially in the fields of crystal engineering (Moghimi *et al.*, 2002; Aghabozorg *et al.*, 2005). We are interested in utilizing 2-(2-pyridyl)imidazole (*L*) as a bidentate chelating ligand to prepare new coordination compounds with intermolecular hydrogen bonds. We report here the structure of the title compound, (I).



(I)

In (I), the metal ion, located on a twofold axis, shows a slightly distorted octahedral geometry with two bidentate chelating ligands *L* and two Cl^- anions in a *cis* arrangement (Fig. 1). The Zn—N distances of 2.070 (2) and 2.310 (2) Å and the Zn—Cl distance of 2.4463 (9) Å are near to the values found in related zinc compounds with this kind of bidentate chelating ligand (Drew *et al.*, 2004). The imidazole H atom forms a hydrogen bond with the Cl atom of an adjacent molecule, generating a two-dimenstional layer structure, as shown in Fig. 2.

Experimental

A mixture of $ZnCl_2\cdot 2H_2O$ (0.017 g, 0.1 mmol), *L* (0.029 g, 0.2 mmol) and water (10 ml) was stirred for 20 min in air. The mixture was

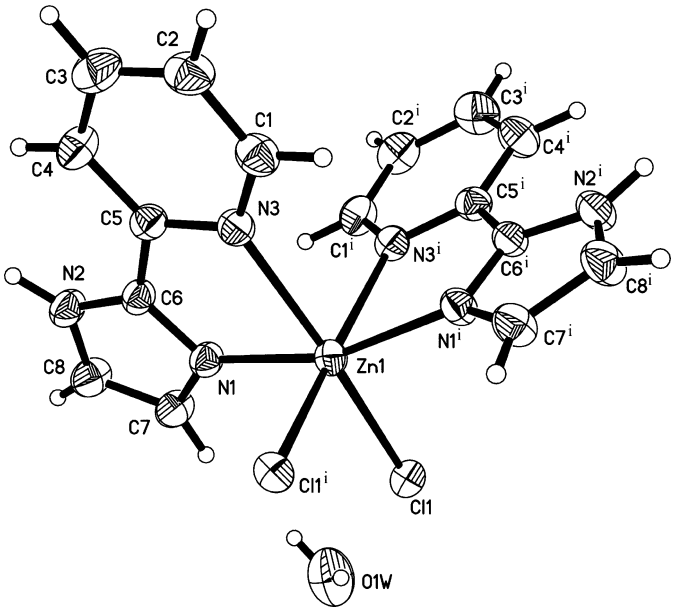


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) $x, -y+\frac{1}{2}, -z+\frac{1}{2}$.]

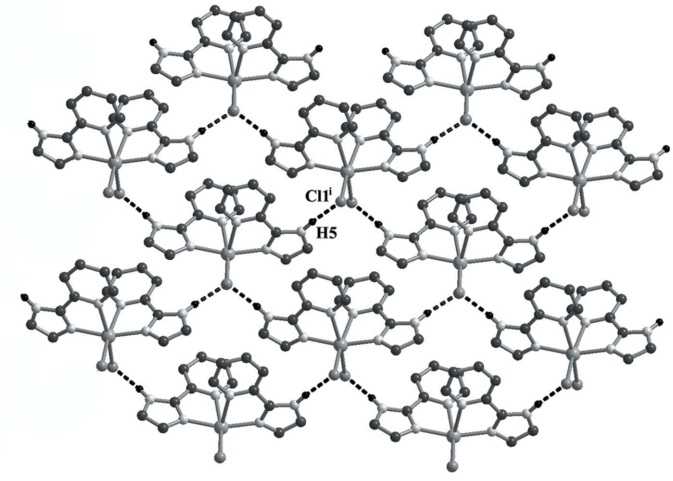


Figure 2
Two-dimensional layer in (I), formed by hydrogen-bonding interactions (dashed lines). [Symmetry code: (i) $x-\frac{1}{2}, \frac{1}{2}-y, z-\frac{1}{2}$.]

transferred to a 23 ml Teflon-lined reactor and kept at 423 K for 3 d under autogenous pressure, and then cooled to room temperature at a rate of 5 K h^{-1}. Colorless crystals were obtained, washed with distilled water and dried at room temperature (yield 60% based on Zn). Analysis caculated for $C_{16}H_{15}Cl_2N_6O_{0.5}Zn$: C 44.32, H 3.49, N 19.38%; found: C 44.33, H 3.49, N 19.39%.

Crystal data

$[ZnCl_2(C_8H_7N_3)_2]\cdot 0.5H_2O$
$M_r = 435.62$
Orthorhombic, *Pnna*
$a = 9.279$ (5) Å
$b = 16.055$ (5) Å
$c = 12.474$ (5) Å
$V = 1858.3$ (14) Å^3
$Z = 4$
$D_x = 1.557$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.62$ mm^{-1}
$T = 293$ (2) K
Block, colorless
0.32 × 0.29 × 0.28 mm

Data collection

Bruker APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.210$, $T_{max} = 0.218$
10539 measured reflections
2222 independent reflections
1740 reflections with $I > 2\sigma(I)$
$R_{int} = 0.049$
$\theta_{max} = 28.3°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.091$
$S = 1.05$
2222 reflections
130 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0581P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.40$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0031 (6)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H5···Cl1^{i}	0.91 (2)	2.25 (2)	3.151 (2)	174.3 (18)

Symmetry code: (i) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$.

All C-bound H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. H atoms on the imidazole N atom and the disordered water molecule were located in a difference Fourier map and refined isotropically, with $U_{iso}(H) = 1.5U_{eq}(N,O)$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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References

Aghabozorg, H., Akbari Saei, A. & Ramezanipour, F. (2005). *Acta Cryst.* E**61**, o3242–o3244.
Bruker (1997). *SMART*. Version 5.622. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SAINT*. Version 6.02. Bruker AXS Inc., Madison, Wisconsin, USA.
Drew, M. G. B., Tocher, D. A., Chowdhury, K., Chowdhury, S. & Datta, D. (2004). *New J. Chem.* **28**, 323–325.
Lan, Y.-Q., Fu, Y.-M., Shao, K.-Z. & Su, Z.-M. (2006). *Acta Cryst.* E**62**, m2586–m2587.
Moghimi, A., Ranibar, M., Aghabozorg, H., Jalali, F., Shamsipur, M., Yap, G. P. A. & Rahbarnoohi, H. (2002). *J. Mol. Struct.* **605**, 133–149.
Sheldrick, G. M. (1990). *SHELXTL-Plus*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Zhang, X. M., Tong, M. L., Gong, M. L. & Chen, X. M. (2003). *Eur. J. Inorg. Chem.* pp. 138–142.