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Key indicators

Single-crystal X-ray study
 $T = 294$ K
Mean $\sigma(\text{C}-\text{C}) = 0.006$ Å
 R factor = 0.037
 wR factor = 0.062
Data-to-parameter ratio = 17.4For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

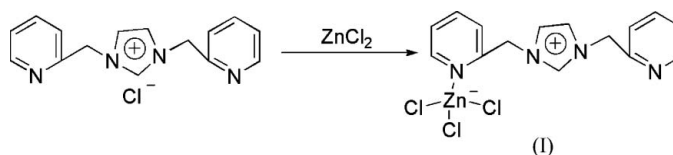
Trichloro[1,3-bis(2-pyridylmethyl)imidazolium]zinc(II)

In the title compound, $[\text{Zn}(\text{C}_{15}\text{H}_{15}\text{N}_4)\text{Cl}_3]$, the Zn^{II} atom is in a distorted tetrahedral environment, coordinated by three Cl atoms and a pyridine N atom. In the crystal packing, the molecules are linked by $\text{C}-\text{H}\cdots\text{Cl}$ hydrogen bonds into a sheet-like structure parallel to the ac plane.

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Comment

Since the discovery of stable imidazolin-2-ylenes by Arduengo *et al.* (1991), much interest has been focused on the chemistry of *N*-heterocyclic carbenes (NHCs) and their metal complexes. In recent years, a number of metal complexes incorporating novel mono-, bi- and tridentate carbene ligands have been synthesized and structurally investigated. Transition metal complexes of chelating carbene ligands containing pyridine units have received a lot of attention owing to their potential applications in organometallic chemistry and homogeneous catalysis (Chen & Lin, 2000; Danopoulos *et al.*, 2003; Poyatos *et al.*, 2003). As a functionalized imidazolium salt, 1,3-di(2-picolyl)imidazolium chloride and its palladium carbene complexes have been prepared and structurally investigated (Magill *et al.*, 2001). Recently, the structures of mono- and trinuclear silver, heteronuclear silver and gold, and mononuclear mercury carbene complexes have been reported (Catalano *et al.*, 2004). Here, the structure of a Zn^{II} complex of 1,3-di(2-picolyl)imidazolium chloride, (I), is presented.



The Zn^{II} atom is in a distorted tetrahedral environment, coordinated by three Cl atoms and a pyridine N atom (Fig. 1). The bond angles around the metal atom range from 105.14 (8) to 114.22 (4) $^\circ$ (Table 1). The planes through the N3/C5–C9 and N4/C11–C15 pyridine rings form dihedral angles of 84.1 (1) and 70.8 (1) $^\circ$, respectively, with the central five-membered ring. The crystal structure is stabilized by $\text{C}-\text{H}\cdots\text{Cl}$ hydrogen bonds (Table 2). The hydrogen bonds link the molecules into a sheet-like structure parallel to the ac plane.

Experimental

1,3-Di(2-picolyl)imidazolium chloride (0.286 g, 1.0 mmol) was added to a solution of anhydrous ZnCl_2 (0.136 g, 1.0 mmol) in methanol (20 ml) at room temperature to obtain compound (I) as a pale brown powder (yield: 90%). Single crystals were grown by slow evaporation of a methanol solution. Analysis calculated for $\text{C}_{15}\text{H}_{15}\text{Cl}_3\text{N}_4\text{Zn}$: C 42.59, H 3.57, N 13.24%; found: C 42.49, H 3.65, N 13.32%. ^1H

NMR(δ , p.p.m.): 9.39 (s, 1H), 8.52 (s, 2H), 7.78–7.89 (m, 4H), 7.36–7.47 (m, 4H), 5.58–5.59 (d, 4H).

Crystal data

[Zn(C₁₅H₁₅N₄)Cl₃]

$M_r = 423.03$

Orthorhombic, $P2_12_12_1$

$a = 8.3222$ (12) Å

$b = 13.3871$ (18) Å

$c = 15.977$ (2) Å

$V = 1780.0$ (4) Å³

$Z = 4$

$D_x = 1.579$ Mg m⁻³

Mo $K\alpha$ radiation

Cell parameters from 2564

reflections

$\theta = 2.8$ – 22.6°

$\mu = 1.83$ mm⁻¹

$T = 294$ (2) K

Block, brown

$0.22 \times 0.16 \times 0.14$ mm

Data collection

Bruker SMART CCD area-detector diffractometer

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.650$, $T_{\max} = 0.774$

10139 measured reflections

3615 independent reflections

2630 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.047$

$\theta_{\text{max}} = 26.4^\circ$

$h = -10 \rightarrow 10$

$k = -11 \rightarrow 16$

$l = -19 \rightarrow 19$

Refinement

Refinement on F^2

$R[F^2 > 2\sigma(F^2)] = 0.037$

$wR(F^2) = 0.062$

$S = 0.99$

3615 reflections

208 parameters

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0127P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.001$

$\Delta\rho_{\text{max}} = 0.34$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.25$ e Å⁻³

Absolute structure: Flack (1983);

1529 Friedel pairs

Flack parameter: -0.015 (13)

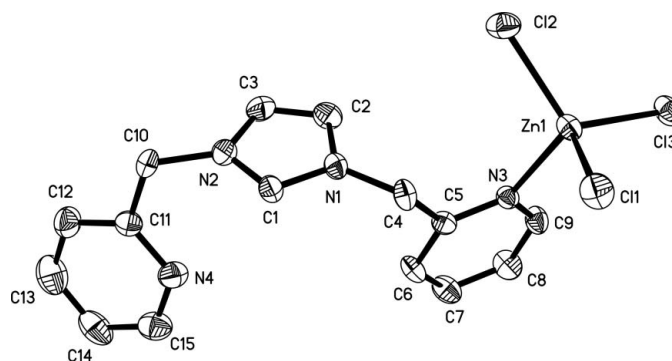


Figure 1

The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. H atoms have been omitted for clarity.

The H atoms were placed in calculated positions, with C–H = 0.93 (aromatic) or 0.97 Å (methylene), and included in the final cycles of refinement using a riding-model approximation, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier atom})$.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Bruker, 1999); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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Table 1

Selected geometric parameters (Å, °).

Zn1–N3	2.099 (3)	Zn1–Cl1	2.2424 (11)
Zn1–Cl2	2.2393 (11)	Zn1–Cl3	2.2548 (11)
N3–Zn1–Cl2	107.64 (8)	N3–Zn1–Cl3	105.14 (8)
N3–Zn1–Cl1	104.47 (8)	Cl2–Zn1–Cl3	113.48 (4)
Cl2–Zn1–Cl1	114.22 (4)	Cl1–Zn1–Cl3	111.00 (4)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C1–H1 \cdots Cl2 ⁱ	0.93	2.83	3.608 (4)	142
C4–H4A \cdots Cl3 ⁱ	0.97	2.83	3.638 (3)	142
C4–H4B \cdots Cl2	0.97	2.74	3.588 (4)	146
C9–H9 \cdots Cl3	0.93	2.78	3.442 (4)	129
C10–H10B \cdots Cl2	0.97	2.80	3.573 (4)	137

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

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