

Dichloridobis(pyridine-3-carbaldehyde- κ N)zinc(II)

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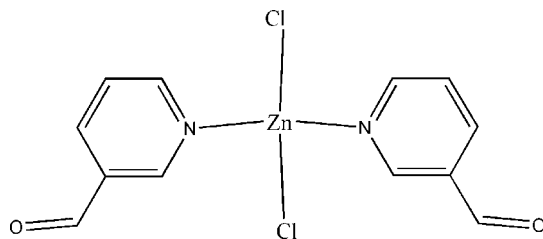
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.022; wR factor = 0.061; data-to-parameter ratio = 18.0.

In the title compound, $[\text{ZnCl}_2(\text{C}_6\text{H}_5\text{NO})_2]$, the Zn^{II} atom lies on a mirror plane, and is coordinated by two N atoms from two pyridine-3-carbaldehyde ligands and two Cl ligands in a distorted tetrahedral geometry. The packing is governed by intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen-bonding interactions.

Related literature

Similar complexes have been previously prepared and studied by Ide *et al.* (2002); Lynton & Sears (1971); Qin *et al.* (1999); Steffen & Palenik (1977).



Experimental

Crystal data

$[\text{ZnCl}_2(\text{C}_6\text{H}_5\text{NO})_2]$	$V = 1382.89$ (4) Å ³
$M_r = 350.49$	$Z = 4$
Orthorhombic, $Pnma$	Mo $K\alpha$ radiation
$a = 5.8445$ (1) Å	$\mu = 2.16$ mm ⁻¹
$b = 19.2032$ (3) Å	$T = 296$ (2) K
$c = 12.3216$ (2) Å	$0.20 \times 0.18 \times 0.18$ mm

Data collection

Bruker APEXII area-detector diffractometer	11915 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	1639 independent reflections
$T_{\text{min}} = 0.659$, $T_{\text{max}} = 0.682$	1412 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.022$	91 parameters
$wR(F^2) = 0.061$	H-atom parameters constrained
$S = 1.05$	$\Delta\rho_{\text{max}} = 0.24$ e Å ⁻³
1639 reflections	$\Delta\rho_{\text{min}} = -0.26$ e Å ⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C3}-\text{H3}\cdots\text{O1}^{\text{i}}$	0.93	2.49	3.342 (2)	152
$\text{C4}-\text{H4}\cdots\text{O1}^{\text{ii}}$	0.93	2.66	3.562 (2)	164

Symmetry codes: (i) $-x + 2, -y + 1, -z$; (ii) $-x + \frac{3}{2}, -y + 1, z - \frac{1}{2}$.

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: XP in SHELXTL (Bruker, 2004); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2084).

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supplementary materials

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Comment

Coordination compounds of the type ZnL_2Cl_2 ($L = 2-NH_2py$, $4-CNpy$, $4-CH_3py$, $4-CH_3COpy$, $3-NH_2COpy$, *etc* (py = pyridine)) have been previously prepared and studied by several groups (Qin *et al.*, 1999; Steffen & Palenik, 1977; Lynton & Sears, 1971; Ide *et al.*, 2002). In this paper, we report the crystal structure of the new mononuclear zinc complex $Zn(3-CHOpy)_2Cl_2$ (where 3-CHOpy is 3-pyridinecarboxaldehyde or nicotinaldehyde).

As illustrated in Fig. 1, the Zn^{II} centre lies on a symmetry plane, defined by the zinc atom and the two chlorine atoms. The zinc center is coordinated to two N atoms from two 3-pyridinecarboxaldehyde ligands and two Cl atoms, and displays a distorted tetrahedral geometry. In the packing, C—H \cdots O hydrogen bonding interactions (Table 1) stabilize the structural components (Fig. 2).

Experimental

The title compound was prepared by the addition of $ZnCl_2$ (1.0 mmol) to an ethanol solution (20 ml) of pyridine-3-carbaldehyde (nicotinaldehyde, 2.0 mmol). The mixture was stirred at 80°C for 2 h and filtered. Colorless prismatic single crystals were obtained from the filtrate upon slow evaporation of the solvent over several days.

Refinement

All H atoms on aromatic rings were placed in calculated positions (C—H = 0.93 Å) and were refined using a riding model with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

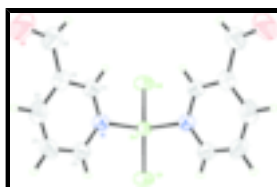


Fig. 1. The molecular structure of the title complex, showing 50% probability displacement ellipsoids. Unlabelled atoms are related to the labelled atoms by the symmetry operator ($x, 1.5 - y, z$).

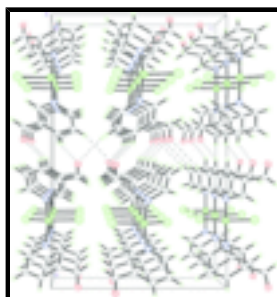


Fig. 2. Packing diagram of the title complex, viewed along the a axis. Dashed lines indicate the C—H \cdots O hydrogen bonds.

Dichloridobis(pyridine-3-carbaldehyde- κ N)zinc(II)

Crystal data

$[\text{ZnCl}_2(\text{C}_6\text{H}_5\text{NO})_2]$	$F_{000} = 704$
$M_r = 350.49$	$D_x = 1.683 \text{ Mg m}^{-3}$
Orthorhombic, $Pnma$	Mo $K\alpha$ radiation
Hall symbol: -P 2ac 2n	$\lambda = 0.71073 \text{ \AA}$
$a = 5.8445 (1) \text{ \AA}$	Cell parameters from 1650 reflections
$b = 19.2032 (3) \text{ \AA}$	$\theta = 1.4\text{--}28.0^\circ$
$c = 12.3216 (2) \text{ \AA}$	$\mu = 2.16 \text{ mm}^{-1}$
$V = 1382.89 (4) \text{ \AA}^3$	$T = 296 (2) \text{ K}$
$Z = 4$	Prismatic, colourless
	$0.20 \times 0.18 \times 0.18 \text{ mm}$

Data collection

Bruker APEXII area-detector diffractometer	1639 independent reflections
Radiation source: fine-focus sealed tube	1412 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.027$
$T = 296(2) \text{ K}$	$\theta_{\text{max}} = 27.5^\circ$
φ and ω scans	$\theta_{\text{min}} = 2.0^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -7 \rightarrow 7$
$T_{\text{min}} = 0.659$, $T_{\text{max}} = 0.682$	$k = -24 \rightarrow 23$
11915 measured reflections	$l = -14 \rightarrow 16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.022$	H-atom parameters constrained
$wR(F^2) = 0.061$	$w = 1/[\sigma^2(F_o^2) + (0.0316P)^2 + 0.3618P]$
$S = 1.05$	where $P = (F_o^2 + 2F_c^2)/3$
1639 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
91 parameters	$\Delta\rho_{\text{max}} = 0.24 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.26 \text{ e \AA}^{-3}$
	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations

between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.4874 (3)	0.65200 (8)	0.05903 (13)	0.0386 (4)
H1	0.4698	0.6765	0.1236	0.046*
C2	0.6525 (3)	0.60094 (9)	0.05413 (15)	0.0420 (4)
C3	0.6773 (3)	0.56404 (9)	-0.04233 (17)	0.0515 (5)
H3	0.7865	0.5290	-0.0483	0.062*
C4	0.5380 (4)	0.58012 (9)	-0.12864 (15)	0.0516 (5)
H4	0.5512	0.5560	-0.1938	0.062*
C5	0.3783 (3)	0.63254 (9)	-0.11717 (14)	0.0450 (4)
H5	0.2860	0.6436	-0.1762	0.054*
C6	0.7926 (3)	0.58667 (10)	0.15072 (16)	0.0542 (5)
H6	0.7659	0.6133	0.2125	0.065*
Cl1	-0.12237 (11)	0.7500	-0.14568 (5)	0.05127 (17)
Cl2	0.00885 (11)	0.7500	0.15928 (5)	0.05020 (17)
N1	0.3506 (2)	0.66815 (7)	-0.02492 (11)	0.0368 (3)
O1	0.9395 (3)	0.54290 (8)	0.15522 (14)	0.0800 (5)
Zn1	0.12503 (4)	0.7500	-0.01246 (2)	0.03558 (10)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0421 (9)	0.0379 (9)	0.0360 (8)	0.0006 (7)	-0.0002 (7)	-0.0014 (6)
C2	0.0414 (9)	0.0367 (8)	0.0479 (9)	0.0022 (7)	0.0022 (7)	0.0041 (7)
C3	0.0547 (11)	0.0388 (9)	0.0610 (11)	0.0089 (8)	0.0137 (9)	-0.0008 (8)
C4	0.0683 (12)	0.0435 (10)	0.0429 (10)	0.0012 (9)	0.0087 (9)	-0.0087 (8)
C5	0.0541 (11)	0.0441 (9)	0.0369 (8)	-0.0041 (8)	-0.0010 (7)	-0.0015 (7)
C6	0.0513 (11)	0.0511 (11)	0.0601 (11)	0.0052 (9)	-0.0048 (9)	0.0071 (9)
Cl1	0.0436 (4)	0.0672 (4)	0.0430 (3)	0.000	-0.0112 (3)	0.000
Cl2	0.0504 (4)	0.0647 (4)	0.0355 (3)	0.000	0.0057 (3)	0.000
N1	0.0385 (7)	0.0361 (7)	0.0359 (7)	0.0005 (6)	0.0002 (5)	-0.0009 (5)
O1	0.0728 (10)	0.0789 (11)	0.0884 (12)	0.0346 (9)	-0.0138 (9)	0.0078 (9)
Zn1	0.03358 (17)	0.03874 (16)	0.03444 (15)	0.000	-0.00213 (10)	0.000

Geometric parameters (\AA , $^\circ$)

C1—N1	1.344 (2)	C5—N1	1.336 (2)
C1—C2	1.377 (2)	C5—H5	0.9300
C1—H1	0.9300	C6—O1	1.203 (2)
C2—C3	1.391 (3)	C6—H6	0.9300

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C2—C6	1.471 (3)	Cl1—Zn1	2.1876 (7)
C3—C4	1.374 (3)	Cl2—Zn1	2.2223 (6)
C3—H3	0.9300	N1—Zn1	2.0571 (14)
C4—C5	1.380 (3)	Zn1—N1 ⁱ	2.0571 (14)
C4—H4	0.9300		
N1—C1—C2	123.20 (15)	C4—C5—H5	118.6
N1—C1—H1	118.4	O1—C6—C2	124.41 (19)
C2—C1—H1	118.4	O1—C6—H6	117.8
C1—C2—C3	118.24 (17)	C2—C6—H6	117.8
C1—C2—C6	119.17 (17)	C5—N1—C1	117.67 (15)
C3—C2—C6	122.58 (17)	C5—N1—Zn1	122.16 (12)
C4—C3—C2	119.00 (17)	C1—N1—Zn1	120.02 (11)
C4—C3—H3	120.5	N1 ⁱ —Zn1—N1	99.65 (8)
C2—C3—H3	120.5	N1 ⁱ —Zn1—Cl1	111.56 (4)
C3—C4—C5	119.03 (17)	N1—Zn1—Cl1	111.56 (4)
C3—C4—H4	120.5	N1 ⁱ —Zn1—Cl2	105.48 (4)
C5—C4—H4	120.5	N1—Zn1—Cl2	105.48 (4)
N1—C5—C4	122.85 (17)	Cl1—Zn1—Cl2	120.83 (3)
N1—C5—H5	118.6		

Symmetry codes: (i) $x, -y+3/2, z$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C3—H3 \cdots O1 ⁱⁱ	0.93	2.49	3.342 (2)	152
C4—H4 \cdots O1 ⁱⁱⁱ	0.93	2.66	3.562 (2)	164

Symmetry codes: (ii) $-x+2, -y+1, -z$; (iii) $-x+3/2, -y+1, z-1/2$.

Fig. 1

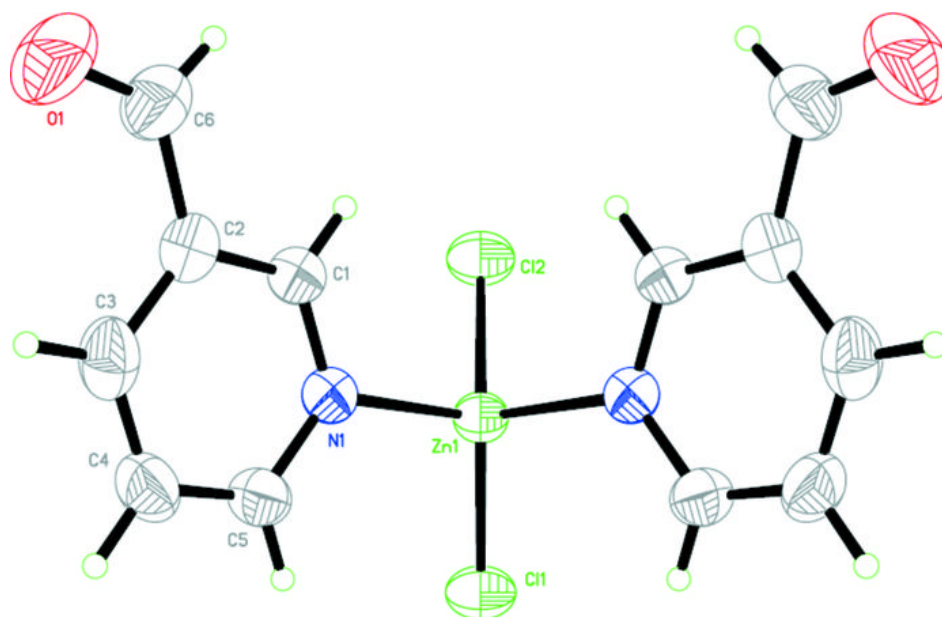


Fig. 2

