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Dichlorido(pyridine-κ*N*)[2-(pyridinium-1-yl)acetato-κ*O*]zinc(II)

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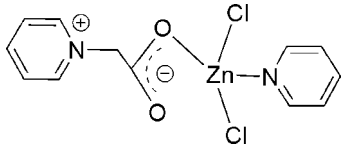
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.014 Å; R factor = 0.073; wR factor = 0.233; data-to-parameter ratio = 19.4.

In the title complex, $[ZnCl_2(C_5H_5N)(C_7H_7NO_2)]$, the Zn^{II} atom adopts a distorted tetrahedral coordination geometry [the smallest angle being 105.22 (15)° and the widest angle being 115.60 (16)°] that is formed from one monodentate carboxylate ligand, one pyridine ligand and two Cl atoms.

Related literature

For background to metalloenzymes, see: Holm & Solomon (2004), Karambelkar *et al.* (2002).



Experimental

Crystal data

$[ZnCl_2(C_5H_5N)(C_7H_7NO_2)]$
M_r = 352.51
Monoclinic, $P2_1/c$
a = 9.979 (2) Å
b = 13.462 (3) Å
c = 13.900 (5) Å
β = 128.781 (19)°
V = 1455.6 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.05 mm^{-1}
T = 291 K
0.48 × 0.36 × 0.32 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*REQAB*; Jacobson, 1998)
T_{min} = 0.439, T_{max} = 0.560
14915 measured reflections
3330 independent reflections
2758 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.073
$wR(F^2)$ = 0.233
S = 1.05
3330 reflections
172 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.96 e Å^{-3}
$\Delta\rho_{min}$ = −1.22 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—O1	1.986 (5)	Zn1—Cl1	2.2884 (18)
Zn1—N2	2.054 (5)	Zn1—Cl2	2.2908 (15)

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL/PC* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL/PC* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FF2059).

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supporting information

Acta Cryst. (2012). E**68**, m485 [https://doi.org/10.1107/S1600536812011749]

Dichlorido(pyridine-*κN*)[2-(pyridinium-1-yl)acetato-*κO*]zinc(II)

Zhang Qun and Chen Jin-Xiang

S1. Comment

The study of synthetic active site analogues has made vast contribution to the understanding of the structure function relationship of many metalloenzymes (Holm *et al.*, 2004). Since the coordination environment of many metalloenzyme active sites is made up of different donor groups, the interest of synthetic chemists has shifted toward the design of mixed ligands (Karambelkar *et al.*, 2002). The title complex (I), has been prepared with the aim to mimic the structures and functions of the active sites of zinc metalloenzymes by using carboxylate ligand and pyridine ligand.

Complex (I) crystallizes in the monoclinic space group P21/c and the asymmetric unit contains one [$C_{12}H_{12}Cl_2N_2O_2Zn$] molecule (Figure 1). In the complex (I), the Zn atom is coordinated one monodentate carboxylate ligand, one pyridine group and two Cl atoms, hence forming a distorted tetrahedral geometry.

S2. Experimental

The title complex was synthesized by reaction of *N*-(carboxymethyl)pyridinium bromide (1.09 g, 5 mmol) and $ZnCl_2$ (0.68 g, 5 mmol) in pyridine (10 ml). The solution was stirred for 2 h to afford white precipitates. The precipitates were collected by filtration, re-dissolved in H_2O (5 ml) then allowed to stand for several days to produce white crystals (I). Yield: 1.53 g (87%). The crystal used for the crystal structure determination was obtained directly from the above preparation. Analysis, found: C, 40.32; H, 3.31; N, 7.62%. calculated. for $C_{12}H_{12}Cl_2N_2O_2Zn$: C, 40.76; H, 3.71; N, 7.92%.

S3. Refinement

Carbon-bond H atoms were positioned geometrically (C—H = 0.93 Å for phenyl group), and were included in the refinement in the riding model approximation, with U_{iso}(H) = 1.2U_{eq}(C).

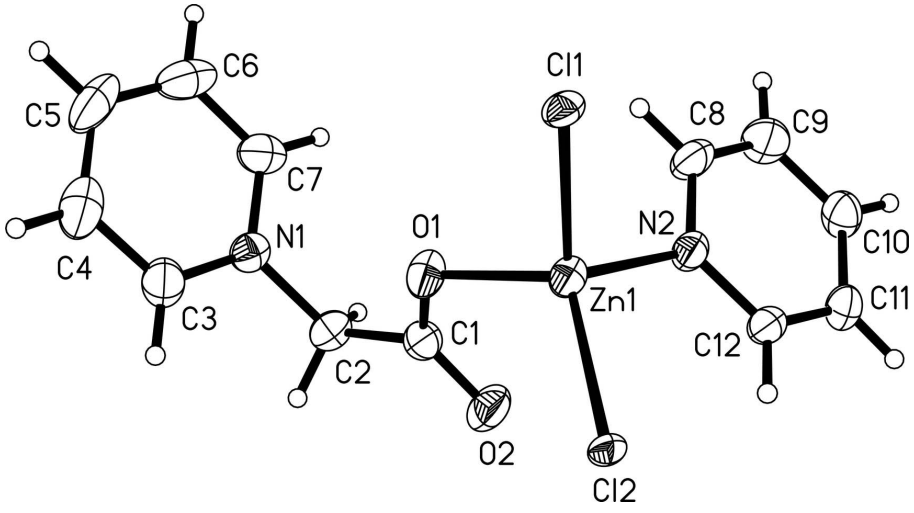

Figure 1

Ellipsoid plot of complex (I) at the 30% probability level. Hydrogen atoms are drawn as spheres of arbitrary radii.

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Crystal data

$[ZnCl_2(C_5H_5N)(C_7H_7NO_2)]$
$M_r = 352.51$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 9.979$ (2) Å
$b = 13.462$ (3) Å
$c = 13.900$ (5) Å
$\beta = 128.781$ (19)°
$V = 1455.6$ (7) Å^3
$Z = 4$
$F(000) = 712$
$D_x = 1.609$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 15259 reflections
$\theta = 3.0$–27.5°
$\mu = 2.05$ mm^{-1}
$T = 291$ K
Prism, colourless
0.48 × 0.36 × 0.32 mm

Data collection

Rigaku SCXmini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*REQAB*; Jacobson, 1998)
$T_{min} = 0.439$, $T_{max} = 0.560$
14915 measured reflections
3330 independent reflections
2758 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.0°$
$h = -12 \rightarrow 12$
$k = -17 \rightarrow 17$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.073$
$wR(F^2) = 0.233$
$S = 1.05$
3330 reflections
172 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1207P)^2 + 8.0068P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.96$ e Å^{-3}
$\Delta\rho_{min} = -1.22$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.42997 (9)	0.41457 (6)	0.23620 (7)	0.0417 (3)
Cl1	0.59745 (17)	0.39808 (11)	0.44591 (12)	0.0375 (4)
Cl2	0.27820 (17)	0.56039 (10)	0.16703 (15)	0.0397 (4)
O1	0.5887 (6)	0.3946 (4)	0.1974 (4)	0.0487 (11)
O2	0.3636 (6)	0.3927 (4)	−0.0052 (5)	0.0609 (14)
N1	0.8205 (7)	0.3545 (4)	0.1608 (5)	0.0430 (12)
N2	0.2623 (6)	0.2967 (4)	0.1606 (5)	0.0418 (12)
C1	0.5189 (8)	0.3845 (5)	0.0830 (6)	0.0420 (14)
C2	0.6349 (8)	0.3582 (5)	0.0525 (6)	0.0465 (15)
H2A	0.6007	0.2938	0.0122	0.056*
H2B	0.6185	0.4065	−0.0058	0.056*
C3	0.9172 (11)	0.4374 (6)	0.1957 (8)	0.0593 (19)
H3A	0.8674	0.4955	0.1502	0.071*
C4	1.0839 (12)	0.4372 (9)	0.2949 (10)	0.079 (3)
H4A	1.1477	0.4954	0.3197	0.095*
C5	1.1604 (11)	0.3512 (10)	0.3600 (8)	0.083 (3)
H5A	1.2768	0.3496	0.4275	0.100*
C6	1.0591 (13)	0.2657 (9)	0.3225 (8)	0.077 (3)
H6A	1.1076	0.2061	0.3648	0.092*
C7	0.8907 (11)	0.2704 (6)	0.2246 (7)	0.0570 (18)
H7A	0.8224	0.2142	0.2010	0.068*
C8	0.3213 (9)	0.2025 (6)	0.2002 (7)	0.0558 (18)
H8	0.4388	0.1923	0.2601	0.067*
C9	0.2123 (11)	0.1218 (6)	0.1544 (9)	0.064 (2)
H9A	0.2561	0.0581	0.1825	0.077*
C10	0.0402 (10)	0.1364 (6)	0.0676 (8)	0.0573 (18)
H10A	−0.0353	0.0830	0.0373	0.069*
C11	−0.0216 (9)	0.2317 (5)	0.0247 (7)	0.0493 (16)
H11A	−0.1386	0.2431	−0.0361	0.059*
C12	0.0944 (8)	0.3094 (5)	0.0742 (6)	0.0426 (14)
H12A	0.0528	0.3734	0.0456	0.051*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0310 (4)	0.0442 (5)	0.0454 (5)	0.0012 (3)	0.0217 (4)	0.0033 (3)

Cl1	0.0289 (7)	0.0449 (8)	0.0263 (6)	0.0031 (5)	0.0112 (5)	0.0024 (5)
Cl2	0.0297 (7)	0.0281 (7)	0.0543 (9)	0.0099 (5)	0.0229 (6)	0.0156 (6)
O1	0.035 (2)	0.066 (3)	0.048 (3)	−0.003 (2)	0.027 (2)	−0.006 (2)
O2	0.036 (3)	0.069 (3)	0.055 (3)	−0.002 (2)	0.018 (2)	−0.003 (3)
N1	0.043 (3)	0.049 (3)	0.042 (3)	0.006 (2)	0.029 (2)	−0.001 (2)
N2	0.034 (3)	0.042 (3)	0.046 (3)	0.001 (2)	0.023 (2)	0.001 (2)
C1	0.038 (3)	0.035 (3)	0.048 (4)	−0.003 (2)	0.024 (3)	0.000 (3)
C2	0.042 (3)	0.047 (4)	0.041 (3)	0.003 (3)	0.021 (3)	−0.003 (3)
C3	0.056 (4)	0.060 (5)	0.065 (5)	−0.009 (4)	0.039 (4)	−0.003 (4)
C4	0.055 (5)	0.099 (8)	0.083 (7)	−0.012 (5)	0.043 (5)	−0.010 (6)
C5	0.037 (4)	0.156 (11)	0.053 (5)	0.008 (6)	0.026 (4)	−0.006 (6)
C6	0.077 (6)	0.105 (8)	0.058 (5)	0.047 (6)	0.047 (5)	0.031 (5)
C7	0.066 (5)	0.059 (5)	0.055 (4)	0.015 (4)	0.043 (4)	0.010 (3)
C8	0.041 (3)	0.051 (4)	0.064 (4)	0.015 (3)	0.027 (3)	0.013 (3)
C9	0.068 (5)	0.039 (4)	0.084 (6)	0.009 (4)	0.047 (5)	0.010 (4)
C10	0.058 (4)	0.044 (4)	0.076 (5)	−0.008 (3)	0.045 (4)	−0.005 (4)
C11	0.041 (3)	0.053 (4)	0.056 (4)	−0.006 (3)	0.030 (3)	−0.004 (3)
C12	0.035 (3)	0.044 (3)	0.043 (3)	0.004 (3)	0.022 (3)	0.006 (3)

Geometric parameters (Å, º)

Zn1—O1	1.986 (5)	C4—C5	1.370 (16)
Zn1—N2	2.054 (5)	C4—H4A	0.9300
Zn1—Cl1	2.2884 (18)	C5—C6	1.399 (16)
Zn1—Cl2	2.2908 (15)	C5—H5A	0.9300
O1—C1	1.283 (8)	C6—C7	1.347 (12)
O2—C1	1.240 (8)	C6—H6A	0.9300
N1—C3	1.352 (10)	C7—H7A	0.9300
N1—C7	1.334 (9)	C8—C9	1.379 (12)
N1—C2	1.485 (8)	C8—H8	0.9300
N2—C12	1.327 (8)	C9—C10	1.359 (12)
N2—C8	1.360 (9)	C9—H9A	0.9300
C1—C2	1.502 (9)	C10—C11	1.386 (11)
C2—H2A	0.9700	C10—H10A	0.9300
C2—H2B	0.9700	C11—C12	1.381 (9)
C3—C4	1.339 (12)	C11—H11A	0.9300
C3—H3A	0.9300	C12—H12A	0.9300
O1—Zn1—N2	106.8 (2)	C5—C4—H4A	120.0
O1—Zn1—Cl1	105.22 (15)	C3—C4—H4A	120.0
N2—Zn1—Cl1	106.73 (16)	C4—C5—C6	118.4 (8)
O1—Zn1—Cl2	115.60 (16)	C4—C5—H5A	120.8
N2—Zn1—Cl2	109.57 (15)	C6—C5—H5A	120.8
Cl1—Zn1—Cl2	112.40 (7)	C7—C6—C5	119.4 (9)
C1—O1—Zn1	116.4 (4)	C7—C6—H6A	120.3
C3—N1—C7	120.2 (7)	C5—C6—H6A	120.3
C3—N1—C2	119.6 (6)	N1—C7—C6	121.0 (9)
C7—N1—C2	120.3 (7)	N1—C7—H7A	119.5

C12—N2—C8	117.9 (6)	C6—C7—H7A	119.5
C12—N2—Zn1	121.7 (5)	N2—C8—C9	122.1 (7)
C8—N2—Zn1	120.4 (5)	N2—C8—H8	118.9
O2—C1—O1	126.0 (6)	C9—C8—H8	118.9
O2—C1—C2	116.7 (6)	C8—C9—C10	119.2 (7)
O1—C1—C2	117.3 (6)	C8—C9—H9A	120.4
N1—C2—C1	114.5 (5)	C10—C9—H9A	120.4
N1—C2—H2A	108.6	C11—C10—C9	119.4 (7)
C1—C2—H2A	108.6	C11—C10—H10A	120.3
N1—C2—H2B	108.6	C9—C10—H10A	120.3
C1—C2—H2B	108.6	C10—C11—C12	118.6 (7)
H2A—C2—H2B	107.6	C10—C11—H11A	120.7
N1—C3—C4	121.0 (9)	C12—C11—H11A	120.7
N1—C3—H3A	119.5	N2—C12—C11	122.9 (6)
C4—C3—H3A	119.5	N2—C12—H12A	118.6
C5—C4—C3	120.1 (10)	C11—C12—H12A	118.6

N2—Zn1—O1—C1	55.9 (5)	C2—N1—C3—C4	178.2 (8)
Cl1—Zn1—O1—C1	169.1 (4)	N1—C3—C4—C5	2.5 (14)
Cl2—Zn1—O1—C1	−66.3 (5)	C3—C4—C5—C6	−2.0 (14)
O1—Zn1—N2—C12	−118.6 (5)	C4—C5—C6—C7	−0.2 (13)
Cl1—Zn1—N2—C12	129.2 (5)	C3—N1—C7—C6	−1.6 (11)
Cl2—Zn1—N2—C12	7.2 (6)	C2—N1—C7—C6	179.6 (7)
O1—Zn1—N2—C8	62.7 (6)	C5—C6—C7—N1	2.0 (12)
Cl1—Zn1—N2—C8	−49.4 (6)	C12—N2—C8—C9	−0.7 (11)
Cl2—Zn1—N2—C8	−171.4 (5)	Zn1—N2—C8—C9	178.0 (7)
Zn1—O1—C1—O2	5.2 (9)	N2—C8—C9—C10	−0.6 (14)
Zn1—O1—C1—C2	−173.4 (4)	C8—C9—C10—C11	1.7 (13)
C3—N1—C2—C1	−90.2 (8)	C9—C10—C11—C12	−1.6 (12)
C7—N1—C2—C1	88.6 (8)	C8—N2—C12—C11	0.8 (10)
O2—C1—C2—N1	176.9 (6)	Zn1—N2—C12—C11	−177.8 (5)
O1—C1—C2—N1	−4.3 (9)	C10—C11—C12—N2	0.3 (11)
C7—N1—C3—C4	−0.6 (12)		