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Diaquabis(5-methylpyridine-2-carboxylato-$\kappa^2 N,O$)zinc(II)

Lian-Cai Du

College of Bioengineering, Weifang University, Weifang 261061, People's Republic of China
Correspondence e-mail: taixishi@lzu.edu.cn

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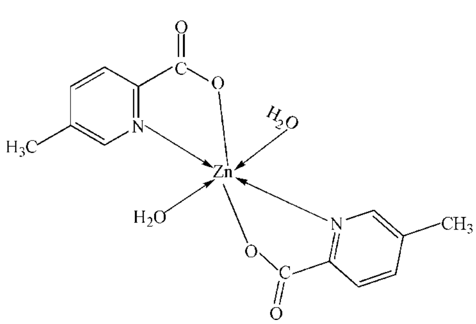
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.034; wR factor = 0.097; data-to-parameter ratio = 11.8.

In the title compound, $[Zn(C_7H_6NO_2)_2(H_2O)_2]$, the Zn atom (site symmetry $\overline{1}$) adopts a distorted *trans*-ZnN_2O_4 octahedral coordination arising from two *N*,*O*-bidentate 5-methylpyridine-2-carboxylate ligands and two water molecules. In the crystal structure, molecules form a layered network linked by O—H$\cdots$O hydrogen bonds.

Related literature

For background, see: Hagrman *et al.* (1998); Ranford *et al.* (1998).



Experimental

Crystal data

$[Zn(C_7H_6NO_2)_2(H_2O)_2]$
M_r = 373.66
Triclinic, $P\overline{1}$
a = 5.1703 (6) Å
b = 6.4620 (10) Å
c = 12.2781 (14) Å
α = 104.678 (2)°
β = 90.646 (1)°
γ = 109.493 (2)°
V = 372.01 (8) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.68 mm^{-1}
T = 298 (2) K
0.49 × 0.46 × 0.27 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.493, T_{max} = 0.659
1917 measured reflections
1275 independent reflections
1260 reflections with $I > 2\sigma(I)$
R_{int} = 0.013

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.097
S = 1.15
1275 reflections
108 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—O1	2.104 (2)	Zn1—N1	2.116 (2)
Zn1—O3	2.134 (2)		

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O3—H3$A\cdots$O2^{i}	0.85	1.88	2.693 (4)	160
O3—H3$B\cdots$O1^{ii}	0.85	1.94	2.757 (3)	160

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $x-1, y, z$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: HB2880).

References

Bruker (2000). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Hagrman, D., Hammond, R. P. & Haushalter, R. (1998). *Chem. Mater.* **10**, 2091–2096.
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supplementary materials

Acta Cryst. (2009). E**65**, m106 [doi:10.1107/S1600536808042530]

Diaquabis(5-methylpyridine-2-carboxylato-κ^2*N*,*O*)zinc(II)

L.-C. Du

Comment

As part of our efforts to achieve supramolecular transition metal complexes by self-assembly (Ranford, *et al.*, 1998; Hagrman, *et al.*, 1998), we now report on the synthesis and crystal structure of the title compound, (I), (Fig. 1).

The Zn^{II} centre in (I) is six-coordinate with two O donors of H_2O, and two N,O-bidentate ligands (Table 1). In the crystal packing, the molecules form a layers linked by O—H···O hydrogen bonds (Table 2).

Experimental

A solution of 1.0 mmol 5-methylpyridine-2-carboxylic acid and 1.0 mmol NaOH in 5 ml 95% ethanol was added to a solution of 0.5 mmol $Zn(CH_3COO)_2.4H_2O$ in 5 ml ethanol at room temperature. The mixture was refluxed for 2 h with stirring, then the resulting precipitate was filtered, washed, and dried *in vacuo* over P_4O_{10} for 48 h. Colourless blocks of (I) were obtained by slowly evaporating from methanol at room temperature.

Refinement

The H atoms were geometrically placed (C—H = 0.93-0.96Å, O—H = 0.85Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}$(C, O) or $1.5U_{eq}$(methyl C).

Figures

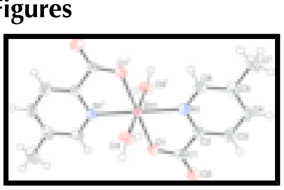

Fig. 1. The molecular structure of (I) showing 50% displacement ellipsoids for the non-hydrogen atoms. Symmetry code: (i) 1–x, 1–y, 1–z.

Diaquabis(5-methylpyridine-2-carboxylato-κ²N,O)zinc(II)

Crystal data

$[Zn(C_7H_6NO_2)_2(H_2O)_2]$	$Z = 1$
$M_r = 373.66$	$F_{000} = 192$
Triclinic, $P\overline{1}$	$D_x = 1.668$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 5.1703 (6)$ Å	Cell parameters from 1975 reflections

b = 6.4620 (10) Å	θ = 3.4–27.9°
c = 12.2781 (14) Å	μ = 1.68 mm^{-1}
α = 104.678 (2)°	T = 298 (2) K
β = 90.646 (1)°	Block, colourless
γ = 109.493 (2)°	0.49 × 0.46 × 0.27 mm
V = 372.01 (8) Å^3	

Data collection

Bruker SMART CCD diffractometer	1275 independent reflections
Radiation source: fine-focus sealed tube	1260 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.013
T = 298(2) K	θ_{max} = 25.0°
ω scans	θ_{min} = 1.7°
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$h = -6 \rightarrow 3$
T_{min} = 0.493, T_{max} = 0.659	$k = -6 \rightarrow 7$
1917 measured reflections	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.034	$w = 1/[\sigma^2(F_o^2) + (0.0603P)^2 + 0.3083P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.097	$(\Delta/\sigma)_{max}$ < 0.001
S = 1.15	$\Delta\rho_{max}$ = 0.63 e Å^{-3}
1275 reflections	$\Delta\rho_{min}$ = −0.60 e Å^{-3}
108 parameters	Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.094 (11)
Secondary atom site location: difference Fourier map	

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Zn1	0.5000	0.5000	0.5000	0.0269 (2)
N1	0.4060 (5)	0.5257 (4)	0.6691 (2)	0.0265 (5)
C4	0.3260 (7)	0.5138 (6)	0.8903 (2)	0.0351 (7)
H4	0.2979	0.5079	0.9643	0.042*
O1	0.6819 (4)	0.2811 (3)	0.54326 (17)	0.0298 (5)
O2	0.7442 (5)	0.1369 (4)	0.6842 (2)	0.0399 (6)
O3	0.1258 (4)	0.2198 (4)	0.4350 (2)	0.0368 (5)
H3A	0.1410	0.0905	0.4068	0.044*
H3B	−0.0199	0.2048	0.4683	0.044*
C1	0.6533 (6)	0.2552 (5)	0.6414 (2)	0.0266 (6)
C2	0.4953 (6)	0.3907 (5)	0.7150 (2)	0.0269 (6)
C3	0.4520 (8)	0.3852 (6)	0.8251 (3)	0.0417 (8)
H3	0.5124	0.2887	0.8550	0.050*
C6	0.2809 (6)	0.6541 (5)	0.7341 (3)	0.0309 (6)
H6	0.2175	0.7490	0.7040	0.037*
C5	0.2430 (6)	0.6500 (6)	0.8452 (3)	0.0351 (7)
C7	0.1086 (8)	0.8011 (7)	0.9188 (3)	0.0500 (9)
H7A	−0.0093	0.7186	0.9650	0.075*
H7B	0.0010	0.8473	0.8718	0.075*
H7C	0.2483	0.9337	0.9664	0.075*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0346 (3)	0.0309 (3)	0.0229 (3)	0.0191 (2)	0.00841 (19)	0.01007 (19)
N1	0.0300 (12)	0.0281 (12)	0.0253 (12)	0.0143 (10)	0.0049 (10)	0.0083 (10)
C4	0.0477 (18)	0.0513 (19)	0.0163 (13)	0.0286 (15)	0.0102 (12)	0.0108 (13)
O1	0.0357 (11)	0.0321 (11)	0.0293 (11)	0.0209 (9)	0.0098 (8)	0.0089 (9)
O2	0.0559 (14)	0.0394 (12)	0.0369 (12)	0.0323 (11)	0.0035 (10)	0.0111 (10)
O3	0.0337 (11)	0.0298 (11)	0.0486 (13)	0.0161 (9)	0.0117 (10)	0.0067 (10)
C1	0.0274 (13)	0.0224 (13)	0.0306 (15)	0.0109 (11)	0.0018 (11)	0.0052 (11)
C2	0.0304 (14)	0.0264 (13)	0.0252 (14)	0.0119 (11)	0.0036 (11)	0.0066 (11)
C3	0.054 (2)	0.051 (2)	0.0337 (17)	0.0306 (17)	0.0084 (15)	0.0194 (15)
C6	0.0349 (15)	0.0321 (15)	0.0313 (15)	0.0196 (12)	0.0078 (12)	0.0076 (12)
C5	0.0341 (15)	0.0399 (17)	0.0289 (15)	0.0146 (13)	0.0065 (12)	0.0029 (13)
C7	0.054 (2)	0.059 (2)	0.0395 (19)	0.0315 (19)	0.0155 (16)	0.0005 (17)

Geometric parameters (Å, °)

Zn1—O1	2.104 (2)	O2—C1	1.232 (4)
Zn1—O3	2.134 (2)	O3—H3A	0.8499
Zn1—O1^{i}	2.104 (2)	O3—H3B	0.8499
Zn1—N1^{i}	2.116 (2)	C1—C2	1.531 (4)
Zn1—N1	2.116 (2)	C2—C3	1.380 (4)

Zn1—O3^{i}	2.134 (2)	C3—H3	0.9300
N1—C6	1.334 (4)	C6—C5	1.387 (5)
N1—C2	1.343 (4)	C6—H6	0.9300
C4—C5	1.327 (5)	C5—C7	1.507 (4)
C4—C3	1.338 (5)	C7—H7A	0.9600
C4—H4	0.9300	C7—H7B	0.9600
O1—C1	1.262 (4)	C7—H7C	0.9600

O1—Zn1—O1^{i}	180.0	Zn1—O3—H3B	121.9
O1—Zn1—N1^{i}	100.78 (8)	H3A—O3—H3B	110.5
O1^{i}—Zn1—N1^{i}	79.22 (8)	O2—C1—O1	126.8 (3)
O1—Zn1—N1	79.22 (8)	O2—C1—C2	117.3 (3)
O1^{i}—Zn1—N1	100.78 (8)	O1—C1—C2	115.9 (2)
N1^{i}—Zn1—N1	180.0	N1—C2—C3	120.1 (3)
O1—Zn1—O3^{i}	89.38 (9)	N1—C2—C1	116.9 (2)
O1^{i}—Zn1—O3^{i}	90.62 (9)	C3—C2—C1	123.0 (3)
N1^{i}—Zn1—O3^{i}	92.23 (9)	C4—C3—C2	122.3 (3)
N1—Zn1—O3^{i}	87.77 (9)	C4—C3—H3	118.8
O1—Zn1—O3	90.62 (9)	C2—C3—H3	118.8
O1^{i}—Zn1—O3	89.38 (9)	N1—C6—C5	121.7 (3)
N1^{i}—Zn1—O3	87.77 (9)	N1—C6—H6	119.1
N1—Zn1—O3	92.23 (9)	C5—C6—H6	119.1
O3^{i}—Zn1—O3	180.0	C4—C5—C6	120.9 (3)
C6—N1—C2	117.7 (2)	C4—C5—C7	117.9 (3)
C6—N1—Zn1	130.4 (2)	C6—C5—C7	121.2 (3)
C2—N1—Zn1	111.95 (18)	C5—C7—H7A	109.5
C5—C4—C3	117.3 (3)	C5—C7—H7B	109.5
C5—C4—H4	121.3	H7A—C7—H7B	109.5
C3—C4—H4	121.3	C5—C7—H7C	109.5
C1—O1—Zn1	115.99 (17)	H7A—C7—H7C	109.5
Zn1—O3—H3A	116.6	H7B—C7—H7C	109.5

O1—Zn1—N1—C6	176.5 (3)	C6—N1—C2—C1	−176.5 (2)
O1^{i}—Zn1—N1—C6	−3.5 (3)	Zn1—N1—C2—C1	2.3 (3)
O3^{i}—Zn1—N1—C6	86.7 (3)	O2—C1—C2—N1	177.6 (3)
O3—Zn1—N1—C6	−93.3 (3)	O1—C1—C2—N1	−0.9 (4)
O1—Zn1—N1—C2	−2.21 (19)	O2—C1—C2—C3	0.0 (4)
O1^{i}—Zn1—N1—C2	177.79 (19)	O1—C1—C2—C3	−178.5 (3)
O3^{i}—Zn1—N1—C2	−92.0 (2)	C5—C4—C3—C2	−0.2 (6)
O3—Zn1—N1—C2	88.0 (2)	N1—C2—C3—C4	−1.1 (5)
N1^{i}—Zn1—O1—C1	−178.1 (2)	C1—C2—C3—C4	176.4 (3)
N1—Zn1—O1—C1	1.9 (2)	C2—N1—C6—C5	0.0 (4)
O3^{i}—Zn1—O1—C1	89.7 (2)	Zn1—N1—C6—C5	−178.6 (2)
O3—Zn1—O1—C1	−90.3 (2)	C3—C4—C5—C6	1.3 (5)
Zn1—O1—C1—O2	−179.4 (2)	C3—C4—C5—C7	−178.2 (3)
Zn1—O1—C1—C2	−1.2 (3)	N1—C6—C5—C4	−1.3 (5)
C6—N1—C2—C3	1.2 (4)	N1—C6—C5—C7	178.2 (3)

Zn1—N1—C2—C3	−180.0 (2)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3A···O2^{ii}	0.85	1.88	2.693 (4)	160
O3—H3B···O1^{iii}	0.85	1.94	2.757 (3)	160

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

Fig. 1