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Poly[*trans*-diaquabis[μ_2-2-(pyridin-3-yl)acetato-κ^2N:O]zinc]

Yue-Hua Li,[a,b] Lin Du,[a] Zong-Ze Li[a] and Qi-Hua Zhao[a]*

[a]School of Chemical Science and Engineering, Yunnan University, Kunming 650091, People's Republic of China, and [b]School of Pharmacy, Dali University, Dali 671000, People's Republic of China
Correspondence e-mail: qhzhao@ynu.edu.cn

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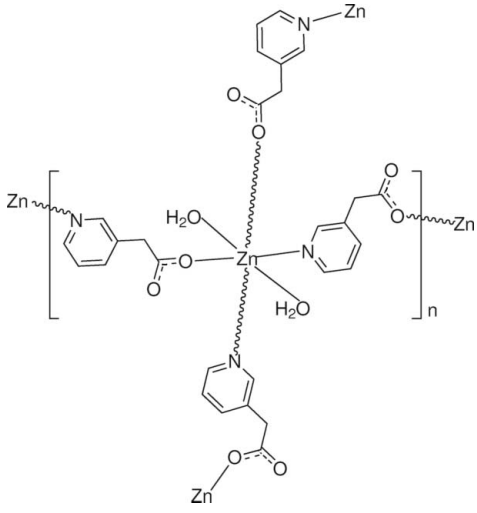
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.042; wR factor = 0.098; data-to-parameter ratio = 15.5.

In the title coordination polymer, $[Zn(C_7H_6NO_2)_2(H_2O)_2]_n$, the Zn^{II} cation is located on an inversion center and is coordinated by four pyridylacetate anions and two water molecules in a distorted ZnN_2O_4 octahedral geometry. The pyridine-N and carboxylate-O atoms of the pyridylacetate anion connect to two Zn^{II} cations, forming a two-dimensional polymeric complex extending parallel to (212). Intermolecular O—H···O and weak C—H···O hydrogen bonding is present in the crystal structure.

Related literature

For related complexes with pyridylacetate ligands, see: Li *et al.* (2004); Du *et al.* (2006); Martin *et al.* (2007); Qin *et al.* (2007); Aakeröy *et al.* (1999); Evans & Lin (2002); Tong *et al.* (2003).



Experimental

Crystal data

$[Zn(C_7H_6NO_2)_2(H_2O)_2]$
M_r = 373.66
Monoclinic, $P2_1/n$
a = 9.175 (2) Å
b = 8.686 (2) Å
c = 9.574 (2) Å
β = 105.928 (3)°
V = 733.8 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.71 mm^{-1}
T = 298 K
0.20 × 0.20 × 0.19 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.718, T_{max} = 0.723
4934 measured reflections
1732 independent reflections
1178 reflections with $I > 2\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.098
S = 1.00
1732 reflections
112 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—N1	2.168 (3)	Zn1—O3	2.125 (2)
Zn1—O2^{i}	2.091 (2)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3B···O1^{i}	0.81 (3)	1.99 (3)	2.739 (4)	152 (4)
O3—H3C···O1^{ii}	0.82 (3)	1.97 (3)	2.764 (4)	161 (3)
C1—H1A···O1^{iii}	0.93	2.54	3.443 (5)	163
C3—H3A···O1^{iv}	0.93	2.50	3.366 (5)	155

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: XU5324).

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supplementary materials

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Poly[*trans*-diaquabis[μ_2-2-(pyridin-3-yl)acetato-κ^2N:*O*]zinc]

Y.-H. Li, L. Du, Z.-Z. Li and Q.-H. Zhao

Comment

The compounds of pyridine-carboxylic acids have been extensively utilized in the preparation of metal complexes due to their versatile coordination modes. Though various metal-pyridinepolycarboxylate complexes have been reported (Evans *et al.*, 2002; Aakeröy *et al.*, 1999; Li *et al.*, 2004; Du *et al.*, 2006), 3-pyridylacetate complexes are rare. Only a few of complexes as nickel, cobalt and copper species have been combined up to now (Martin *et al.*, 2007). In this paper, we described a new two-dimensional coordination polymer, $[Zn(3\text{-pyridylacetato})_2(H_2O)_2]_n$, (I). The molecular structure of the title complex is similar to those previously reported such as $[M(4\text{-pyridylacetato})_2(H_2O)_2]_n$ (*M* = Cu, Co, Mn, Ni, Zn, Cd)(Du *et al.*, 2006; Qin *et al.*, 2007; Tong *et al.*, 2003) and $[M(3\text{-pyridylacetato})_2(H_2O)_2]_n$ (*M* = Ni, Co, Cu) (Martin *et al.*, 2007;). Single-crystal X-ray diffraction analysis shows that the title compound is crystallized in a space group $P2_1/n$. The Zn^{II} center is six-coordinated by two water molecules in the axial positions, two pyridyl nitrogen atoms and two carboxylate oxygen atoms from two 3-pyridylacetate ligands in the plane. Pyridine nitrogen atom and carboxylate oxygen atom of each 3-pyridylacetate anion are connected to one Zn^{II} ions. The coordination geometry of Zn^{II} cation can been described as a distorted octahedral geometry with Zn—N and Zn—O distance range 2.168 (2) Å and 2.091 (3)—2.125 (3) Å, respectively (Fig. 1, Table 1). Four 3-pyridylacetate anionic ligands and four Zn^{II} ions are combined to a tetragon, which is of a side length of 8.653 Å and a diagonal measurement of 14.969*8.686 Å based on the Zn—Zn distances. The tetragon is further extended into a two-dimensional framework structure parallel to (212) with arhombic grid through sharing Zn^{II} ions, 3-pyridylacetate anionic ligands. Adjacent two-dimensional layers are connected by the intermolecular O—H···O and weak C—H···O hydrogen-bonding contacts, forming a three-dimensional framework structure with oxygen as a trifurcated acceptor atom (Fig. 2)

Experimental

A mixture of $Zn(COO)_2.H_2O$ (0.1 mmol), 3-pyridyl acetic acid (0.1 mmol), DMF (5.0 ml) and methanol (10.0 ml) was stirred for 30 min and and the crude product was isolated by filtration. The filtrate was purified by recrystallization from anhydrous methanol and DMF to give (I) as colorless block crystals in 60% yield. An solution of (I) was stood at room temperature, and upon slowly evaporating methanol and DMF from the solution, colorless block crystals suitable for X-ray diffraction analysis were isolated in room temperature three week later.

Refinement

Water H atoms were located in a difference Fourier map and positional parameters were refined, $U_{iso}(H) = 1.2U_{eq}(O)$. Other H atoms were generated geometrically and were included in therefinement in the riding model approximation with C—H = 0.93–0.97 Å, $U_{iso}= 1.2U_{eq}(C)$.

Figures

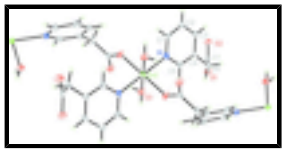

Fig. 1. The molecular structure of the title complex with the atom-numbering diagram. Ellipsoids were drawn at the 30% probability level.

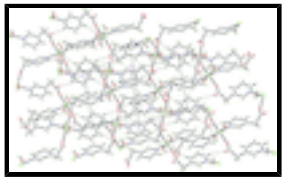

Fig. 2. The packing diagram of (I).

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Crystal data

$[Zn(C_7H_6NO_2)_2(H_2O)_2]$	$F(000) = 384$
$M_r = 373.66$	$D_x = 1.691$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 4934 reflections
$a = 9.175$ (2) Å	$\theta = 3.2$–$28.2°$
$b = 8.686$ (2) Å	$\mu = 1.71$ mm^{-1}
$c = 9.574$ (2) Å	$T = 298$ K
$\beta = 105.928$ (3)°	Block, colorless
$V = 733.8$ (3) Å^3	0.20 × 0.20 × 0.19 mm
$Z = 2$	

Data collection

Bruker APEXII CCD area-detector diffractometer	1732 independent reflections
Radiation source: fine-focus sealed tube	1178 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.054$
φ and ω scans	$\theta_{max} = 28.2°$, $\theta_{min} = 3.2°$
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)	$h = -12 \rightarrow 11$
$T_{min} = 0.718$, $T_{max} = 0.723$	$k = -11 \rightarrow 11$
4934 measured reflections	$l = -9 \rightarrow 12$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.042$	Hydrogen site location: inferred from neighbouring sites

$wR(F^2) = 0.098$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.00$	$w = 1/[\sigma^2(F_o^2) + (0.035P)^2 + 0.2786P]$ where $P = (F_o^2 + 2F_c^2)/3$
1732 reflections	$(\Delta/\sigma)_{max} < 0.001$
112 parameters	$\Delta\rho_{max} = 0.39$ e Å^{-3}
3 restraints	$\Delta\rho_{min} = -0.38$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.5000	0.0000	0.0000	0.02624 (18)
O1	0.2006 (3)	0.1719 (3)	0.6106 (3)	0.0400 (6)
O2	0.0333 (3)	0.2812 (3)	0.4230 (2)	0.0331 (6)
O3	0.6282 (3)	0.0534 (3)	0.2153 (3)	0.0359 (6)
H3C	0.694 (3)	0.002 (3)	0.272 (3)	0.043*
H3B	0.676 (4)	0.130 (3)	0.207 (4)	0.043*
N1	0.3007 (3)	0.0777 (3)	0.0596 (3)	0.0293 (6)
C1	0.1913 (4)	0.1572 (4)	−0.0326 (4)	0.0346 (8)
H1A	0.2032	0.1814	−0.1235	0.042*
C2	0.0611 (4)	0.2054 (4)	0.0003 (4)	0.0372 (9)
H2A	−0.0123	0.2612	−0.0670	0.045*
C3	0.0414 (4)	0.1699 (4)	0.1341 (4)	0.0346 (8)
H3A	−0.0460	0.2004	0.1578	0.042*
C4	0.1537 (4)	0.0881 (4)	0.2333 (3)	0.0267 (7)
C5	0.2802 (4)	0.0449 (4)	0.1900 (4)	0.0295 (8)
H5A	0.3557	−0.0104	0.2555	0.035*
C6	0.1407 (4)	0.0437 (4)	0.3815 (4)	0.0341 (9)
H6A	0.2296	−0.0158	0.4302	0.041*
H6B	0.0532	−0.0229	0.3692	0.041*
C7	0.1255 (4)	0.1768 (4)	0.4799 (4)	0.0278 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0299 (3)	0.0285 (3)	0.0225 (3)	−0.0017 (3)	0.0111 (2)	−0.0004 (2)

O1	0.0477 (16)	0.0369 (14)	0.0309 (14)	0.0064 (12)	0.0033 (12)	0.0006 (11)
O2	0.0417 (15)	0.0324 (13)	0.0259 (12)	0.0088 (11)	0.0106 (11)	−0.0015 (10)
O3	0.0426 (16)	0.0340 (14)	0.0279 (14)	−0.0022 (12)	0.0044 (11)	−0.0018 (11)
N1	0.0336 (17)	0.0316 (16)	0.0256 (15)	−0.0012 (13)	0.0130 (12)	0.0007 (12)
C1	0.045 (2)	0.034 (2)	0.0261 (18)	0.0034 (17)	0.0126 (16)	0.0024 (15)
C2	0.037 (2)	0.039 (2)	0.034 (2)	0.0102 (17)	0.0060 (16)	0.0004 (16)
C3	0.029 (2)	0.037 (2)	0.039 (2)	0.0047 (16)	0.0121 (16)	−0.0065 (17)
C4	0.033 (2)	0.0232 (18)	0.0263 (17)	0.0001 (14)	0.0123 (15)	−0.0021 (14)
C5	0.034 (2)	0.0275 (18)	0.0286 (18)	0.0025 (14)	0.0116 (15)	0.0035 (14)
C6	0.048 (2)	0.0259 (18)	0.035 (2)	0.0059 (16)	0.0234 (17)	0.0035 (14)
C7	0.0286 (19)	0.0282 (18)	0.0314 (19)	−0.0034 (15)	0.0160 (15)	0.0037 (15)

Geometric parameters (Å, °)

Zn1—N1	2.168 (3)	C1—C2	1.382 (5)
Zn1—N1^{i}	2.168 (3)	C1—H1A	0.9300
Zn1—O2^{ii}	2.091 (2)	C2—C3	1.377 (5)
Zn1—O2^{iii}	2.091 (2)	C2—H2A	0.9300
Zn1—O3	2.125 (2)	C3—C4	1.390 (5)
O1—C7	1.252 (4)	C3—H3A	0.9300
O2—C7	1.258 (4)	C4—C5	1.387 (4)
O2—Zn1^{iv}	2.091 (2)	C4—C6	1.507 (4)
O3—H3C	0.825 (18)	C5—H5A	0.9300
O3—H3B	0.812 (17)	C6—C7	1.522 (4)
N1—C1	1.333 (4)	C6—H6A	0.9700
N1—C5	1.344 (4)	C6—H6B	0.9700
O2^{ii}—Zn1—O2^{iii}	180.00 (12)	C1—C2—H2A	120.4
O2^{ii}—Zn1—O3^{i}	87.23 (9)	C2—C3—C4	119.2 (3)
O2^{iii}—Zn1—O3^{i}	92.77 (9)	C2—C3—H3A	120.4
O2^{ii}—Zn1—N1^{i}	88.57 (10)	C4—C3—H3A	120.4
O2^{iii}—Zn1—N1^{i}	91.43 (10)	C5—C4—C3	117.3 (3)
O3^{i}—Zn1—N1^{i}	87.67 (10)	C5—C4—C6	120.1 (3)
O2^{ii}—Zn1—N1	91.43 (10)	C3—C4—C6	122.6 (3)
O2^{iii}—Zn1—N1	88.57 (10)	N1—C5—C4	124.2 (3)
O3^{i}—Zn1—N1	92.33 (10)	N1—C5—H5A	117.9
N1^{i}—Zn1—N1	180.00 (12)	C4—C5—H5A	117.9
C7—O2—Zn1^{iv}	130.4 (2)	C4—C6—C7	115.7 (3)
H3C—O3—H3B	101 (2)	C4—C6—H6A	108.4
C1—N1—C5	117.0 (3)	C7—C6—H6A	108.4
C1—N1—Zn1	121.5 (2)	C4—C6—H6B	108.4
C5—N1—Zn1	121.5 (2)	C7—C6—H6B	108.4
N1—C1—C2	123.1 (3)	H6A—C6—H6B	107.4
N1—C1—H1A	118.4	O1—C7—O2	125.3 (3)
C2—C1—H1A	118.4	O1—C7—C6	118.3 (3)
C3—C2—C1	119.1 (3)	O2—C7—C6	116.4 (3)
C3—C2—H2A	120.4		

Symmetry codes: (i) −*x*+1, −*y*, −*z*; (ii) *x*+1/2, −*y*+1/2, *z*−1/2; (iii) −*x*+1/2, *y*−1/2, −*z*+1/2; (iv) −*x*+1/2, *y*+1/2, −*z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3B···O1^{ii}	0.81 (3)	1.99 (3)	2.739 (4)	152 (4)
O3—H3C···O1^{v}	0.82 (3)	1.97 (3)	2.764 (4)	161 (3)
C1—H1A···O1^{vi}	0.93	2.54	3.443 (5)	163
C3—H3A···O1^{vii}	0.93	2.50	3.366 (5)	155

Symmetry codes: (ii) *x*+1/2, −*y*+1/2, *z*−1/2; (v) −*x*+1, −*y*, −*z*+1; (vi) *x*, *y*, *z*−1; (vii) *x*−1/2, −*y*+1/2, *z*−1/2.

Fig. 1

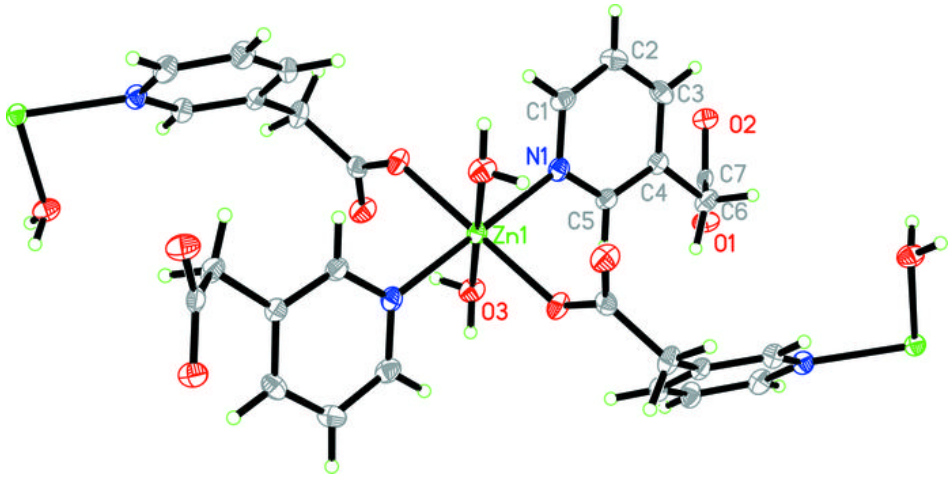

Fig. 2