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catena-Poly[[aquadipyridinezinc(II)]-μ-benzene-1,4-dioxyacetato]

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Key indicators

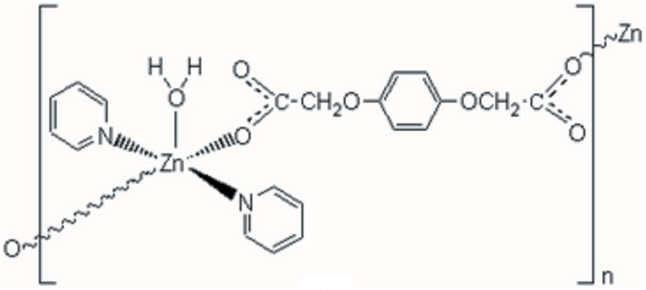
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.042
wR factor = 0.089
Data-to-parameter ratio = 12.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, $\{[Zn(C_{10}H_8O_6)(C_5H_5N)_2(H_2O)]\}_n$, the coordination geometry around the Zn^{II} atom is distorted square-pyramidal, and the $Zn-OH_2$ bond at the apical position lies on a twofold axis. The bis-monodentate benzene-1,4-dioxyacetate ligand has inversion symmetry and acts as a bridge to link Zn atoms to form an infinite zigzag chain. Hydrogen bonds between the coordinated water molecule and the free carboxylate O atoms link the chains along the b axis into a two-dimensional layer.

Comment

Polycarboxylate ligands have attracted considerable attention in the design and synthesis of metal–organic coordination polymers with fascinating architectures and promising applications as porous materials. Interest is stimulated not only by the easy synthesis of various carboxylates, but also by the presence of versatile coordination modes, generally yielding neutral frameworks (Rao *et al.*, 2004). In general, two kinds of bridging ligands have been used, one of which is flexible, such as butanedioic acid and glutaric acid, and the other is rigid, such as benzenedicarboxylate and benzenetricarboxylate. Although many ligands with characteristics of both flexibility and rigidity have been reported, here the ligands refer to those containing both a benzene ring and an aliphatic acid group, reports of which are comparatively rare; these ligands are very important in the development of so-called third-generation coordination polymers with dynamic frameworks and striking functions (Kitagawa *et al.*, 2004). In our group, a series of such ligands have been explored; two of these are benzene-1,4-dioxyacetate and benzene-1,3-dioxyacetate, in which the $-OCH_2$ groups make the ligands more flexible in comparison with benzenedicarboxylates, while the existence of the benzene ring imposes some degree of rigidity. Recently, we have reported a polymeric Cu complex with benzene-1,3-dioxyacetate (Hong *et al.*, 2005). We have further studied the structure of a zinc compound with benzene-1,4-dioxyacetate, which we report here.



(I)

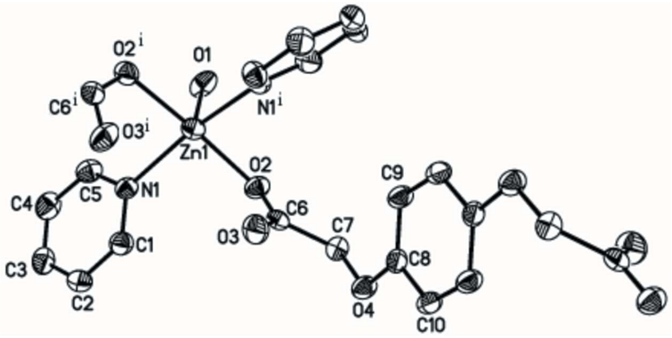


Figure 1
A segment of the polymeric structure of (I), with displacement ellipsoids drawn at the 50% probability level. All H atoms have been omitted for clarity. [Symmetry code: (i) $1 - x, y, \frac{3}{2} - z$.]

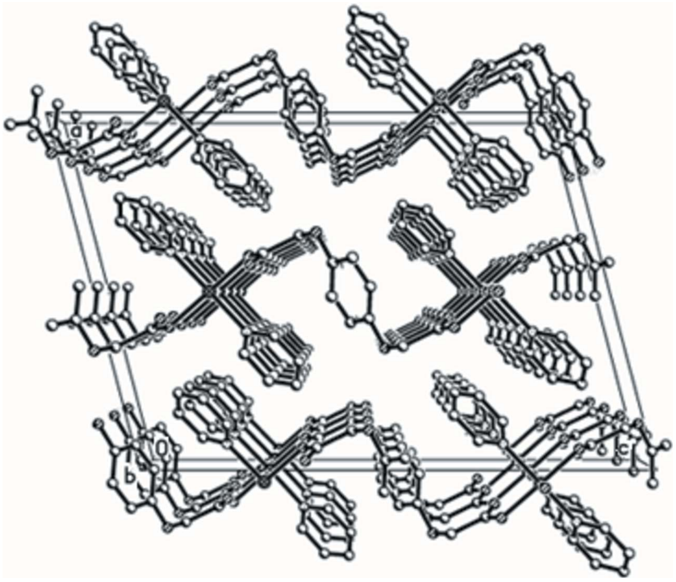


Figure 2
The crystal structure of (I), viewed down the *b* axis. All H atoms have been omitted for clarity.

Although there are 439 structures containing the py–Zn–OOC fragment in the current Cambridge Structural Database (*ConQuest* 1.7; CSD update of May 2005; Allen, 2002), there are no examples involving the benzene-1,4-dioxyacetate ligand. The title complex, (I), a one-dimensional coordination polymer of five-coordinate Zn^{II} cores with benzene-1,4-dioxyacetate and pyridine ligands, is reported here.

The asymmetric unit comprises one Zn^{II} ion on a twofold rotation axis, one pyridine molecule, one-half of a water molecule and one-half of a benzene-1,4-dioxyacetate ligand. The Zn atom is five-coordinated in a distorted square-pyramidal arrangement, with two O atoms of different carboxylate groups and two N atoms of two pyridine ligands in basal positions [N1/N1^i/O2/O2^i; symmetry code: (i) $1 - x, y, \frac{3}{2} - z$] and a water O atom at the apex (O1), as shown in Fig. 1. The Zn1—O1 bond lies on a twofold axis. The bis-monodentate benzene-1,4-dioxyacetate ligand has inversion symmetry and acts as bridge to link the Zn atoms to form an infinite zigzag chain along the *c* axis (Fig. 2), and the distance between two adjacent Zn atoms in the same chain is 10.893 (2) Å (half the length of the *c* axis). It should be noted that the O—H···O hydrogen bonds (Table 2 and Fig. 3), which are between the coordinated water molecule and the free carboxylate O atoms, link the chains into two-dimensional layers.

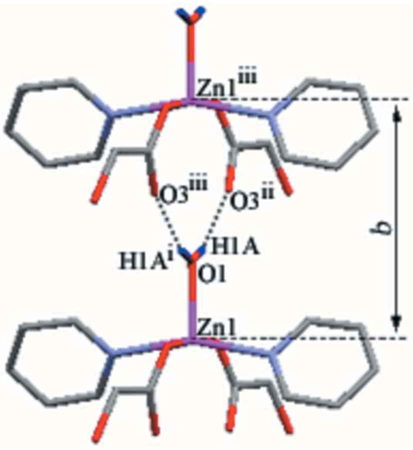


Figure 3
The intermolecular hydrogen bonds along the *b* axis. [Symmetry codes: (i) $1 - x, y, \frac{3}{2} - z$; (ii) $1 - x, 1 + y, \frac{3}{2} - z$; (iii) $x, 1 + y, z$.]

The mean Zn—N and Zn—O distances are comparable with those published for analogous complexes (Yaghi *et al.*, 1997; Darensbourg *et al.*, 2002). It is worth noting that the Zn—OH$_2$ distance is shorter than that in some six-coordinate zinc compounds, such as $[Zn(bipy)_2(H_2O)(CF_3CO_2)](ClO_4)_2$, where there is an N atom *trans* to the water molecule (Ye *et al.*, 1999).

Experimental

Benzene-1,4-dioxyacetic acid was prepared according to the literature (Zhang *et al.*, 2001). 1,4-Benzene-1,4-dioxyacetic acid (0.013 g, 0.05 mmol) and $Zn(ClO_4)_2·6H_2O$ (0.037 g, 0.1 mmol) were dissolved in DMF (10 ml) and placed in a small vial, which was inserted into a larger vial containing pyridine (3 ml). The larger vial was sealed, heated to 333 K and left undisturbed. After 24 h, the larger vial was cooled to room temperature. Several weeks later, yellow crystals of (I) were formed (yield 35%). Analysis calculated for $C_{20}H_{20}N_2O_7Zn$: C 51.57, H 4.33, N 6.01%; found: C 51.79, H 4.46%, N 6.04%. FT–IR (KBr, cm^{-1}): 3383.54 (*m*), 2319.94 (*w*), 1841.29 (*w*), 1618.91 (*vs*), 1600.23 (*vs*), 1508.81 (*s*), 1447.78 (*s*), 1411.48 (*s*), 1341.52 (*m*), 1295.66 (*m*), 1231.85 (*s*), 1217.08 (*v*), 1068.61 (*s*), 829.44 (*m*), 816.43 (*m*), 762.93 (*w*), 695.92 (*s*), 630.60 (*w*).

Crystal data

$[Zn(C_{10}H_8O_6)(C_5H_5N)_2(H_2O)]$
$M_r = 465.75$
Monoclinic, $C2/c$
$a = 15.579\ (3)$ Å
$b = 6.0883\ (12)$ Å
$c = 21.725\ (4)$ Å
$\beta = 104.76\ (3)°$
$V = 1992.6\ (7)$ Å^3
$Z = 4$

$D_x = 1.553$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 2.1–20.5°$
$\mu = 1.28$ mm^{-1}
$T = 293\ (2)$ K
Prism, yellow
0.35 × 0.35 × 0.30 mm

m1864 Hong *et al.* • $[Zn(C_{10}H_8O_6)(C_5H_5N)_2(H_2O)]$ *Acta Cryst.* (2005). E**61**, m1863–m1865

Data collection

Siemens *P*4 diffractometer
$2\theta/\omega$ scans
Absorption correction: ψ scan (*XPREP*; Bruker, 2000)
$T_{\min} = 0.65$, $T_{\max} = 0.68$
4977 measured reflections
1754 independent reflections
1227 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.050$
$\theta_{\max} = 25.0°$
$h = -14 \rightarrow 18$
$k = -7 \rightarrow 7$
$l = -25 \rightarrow 25$
3 standard reflections every 97 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.089$
$S = 0.88$
1754 reflections
138 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0241P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.45$ e Å^{-3}
$\Delta\rho_{\min} = -0.62$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	2.024 (3)	Zn1—N1	2.140 (3)
Zn1—O2	2.040 (2)		
O1—Zn1—O2	92.99 (7)	O2—Zn1—N1	91.26 (10)
O2$^{\text{i}}$—Zn1—O2	174.03 (15)	O2—Zn1—N1$^{\text{i}}$	87.75 (10)
O1—Zn1—N1	99.55 (8)	N1—Zn1—N1$^{\text{i}}$	160.90 (16)

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O3$^{\text{ii}}$	0.82	1.92	2.636 (4)	146

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

H atoms bonded to C atoms were positioned geometrically and refined as riding, with C—H = 0.93–0.97 Å and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The H atom of the water molecule was located in a difference density map, idealized and constrained to maintain ideal geometry, with O—H = 0.82 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$.

Data collection: *XSCANS* (Bruker, 2000); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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