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The one-dimensional zigzag coordination polymer *catena*-poly[[[triaquazinc(II)]-μ-*N*,*N*′-(benzene-1,4-dicarboxamido)diacetato-κ^2*O*:*O*′] dihydrate]

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In the crystal structure of the title compound, $\{[Zn(C_{12}H_{10}N_2O_6)(H_2O)_3]\cdot 2H_2O\}_n$, the Zn^{II} atom is located on a twofold axis and is coordinated by two carboxylate O atoms and three water O atoms in a trigonal-bipyramidal geometry. The diacetate ligands connect Zn^{II} atoms to generate one-dimensional zigzag chains, which are linked together by intermolecular hydrogen bonding to form a three-dimensional supramolecular framework.

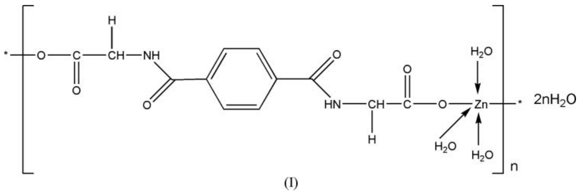
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.042
wR factor = 0.120
Data-to-parameter ratio = 13.0

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

Comment

Considerable effort has been devoted to the design and synthesis of self-assembled coordination polymers owing to their potential applications as functional materials (Janiak, 2003; James, 2003). An emerging approach in the rational assembly of coordination polymers is through the organic ligand as a spacer for linking metal atoms (O′Keeffe *et al.*, 2000). Accordingly, the structures of coordination polymers can be ascribed to the coordination interactions between organic ligands and metal atoms, as well as other non-covalent interactions such as hydrogen bonding and π–π stacking (Moulton & Zaworotko, 2001). Moreover, the conformations of organic ligands also have important influences on the structures. To avoid the structural complication arising from the conformations of the ligands, rigid ligands, such as 1,4-benzenedicarboxylate, are widely employed as spacer linkers (Eddaoudi *et al.*, 2001). Recently, flexible ligands have been used to construct coordination polymers because they may induce some unusual structures (Burrows *et al.*, 2004; Li *et al.*, 2004). However, ligands with both rigidity and flexibility are seldom used to assemble coordination polymers. For example, an *N*-substituted aromatic amide has rigidity owing to the amide group (–CO—N–) conjugating with the aromatic ring, while the σ-rotation about the N—C bond could induce flexibility in the molecule. Moreover, the imine group N—H could serve as a better hydrogen-bonding donor and the amide C═O could also act as a better hydrogen-bonding acceptor (Manoj & Vijayan, 2000). Therefore, we have designed and synthesized a semi-flexible amide ligand, 2,2′-[1,4-bis(-benzamido)]diacetic acid (H_2L), and employed it with Zn^{II} ions to assemble the title coordination polymer, (I).



(I)

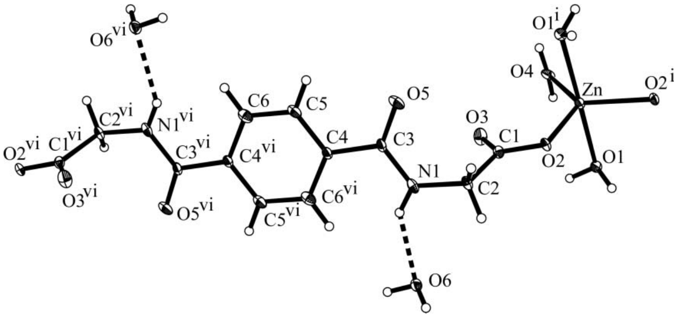


Figure 1
The molecular structure of (I), with displacement ellipsoids at the 25% probability level (arbitrary spheres for H atoms). Dashed lines indicate hydrogen bonds. [Symmetry codes: (i) $2 - x, y, \frac{3}{2} - z$; (vi) $1 - x, -y, 1 - z$.]

As shown in Fig. 1, the asymmetric unit of (I) consists of one-half of a ligand dianion, one-half of a Zn^{II} ion, one and a half coordinated water molecules, and one uncoordinated water molecule. The Zn^{II} and O3 atoms are located on a twofold axis. The Zn^{II} atom is coordinated by five O atoms in a trigonal-bipyramidal geometry, with Zn—O distances ranging from 1.981 (3) to 2.183 (2) Å (Table 1). Two carboxyl O atoms, O2 and O2^{i} [symmetry code: (i) $2 - x, y, \frac{3}{2} - z$], and one water molecule (O4) occupy the equatorial positions, while two water O atoms, O1 and O1^{i}, are located at the axial sites. The axial O1$\cdots$O1^{i} vector is almost perpendicular to the equatorial plane. The C3-amide group is almost coplanar with the benzene ring, while the C1-carboxyl group lies out of the benzamide plane, with a dihedral angle of 74.7 (4)°.

The ligand dianion *L* is located on an inversion center and bridges neighboring Zn^{II} ions to generate one-dimensional zigzag chains propagating along the [201] direction. The small folds near the Zn^{II} ions in the chain can be ascribed to the flexibility arising from rotation about the N—C bond. The C3—N1—C2—C1 torsion angle is −72.7 (4)°.

The dihedral angle between neighboring benzamide planes in the same chain is 68.93 (16)°, and the dihedral angle between the equatorial plane and the benzamide plane is 70.1 (5)°. The Zn$\cdots$Zn intrachain distance is 16.524 (4) Å, while the Zn$\cdots$Zn interchain distance is 5.1898 (8) Å.

All chains are arranged in a parallel fashion. The chains are connected by intermolecular hydrogen bonding to form the three-dimensional supramolecular structure (Fig. 2). The shortest centroid–centroid distance of 5.189 (3) Å between parallel phenyl rings from neighboring chains indicates no π–π stacking interaction (Janiak, 2000). Atom H1*A* is involved in a three-centered hydrogen bond (Table 2).

Experimental

The ligand *L* was synthesized from terephthaloyl chloride and glycine according to a similar method reported by Yuan *et al.* (2002). *L* (28.0 mg, 0.1 mmol) was dissolved in an aqueous solution (10 ml) of $Zn(CH_3COO)_2 \cdot 4H_2O$ (22.0 mg, 0.1 mmol). The resulting colorless solution was filtered and the filtrate was left at room temperature. Colorless platelet crystals of (I) were obtained (20.1 mg, yield *ca* 46%) after several weeks by slow evaporation of the solvent.

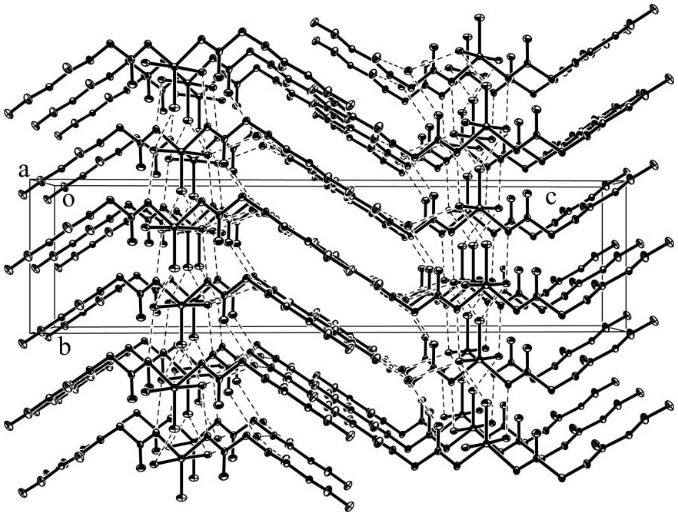


Figure 2
A packing diagram of (I), viewed down the *a* axis. All H atoms have been omitted for clarity. Dashed lines indicate hydrogen bonds.

Crystal data

$[Zn(C_{12}H_{10}N_2O_6)(H_2O)_3] \cdot 2H_2O$
$M_r = 433.69$
Monoclinic, $C2/c$
$a = 6.8980$ (14) Å
$b = 7.7550$ (16) Å
$c = 30.339$ (6) Å
$\beta = 93.44$ (3)°
$V = 1620.0$ (6) Å^3
$Z = 4$

$D_x = 1.778$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 2.5$–15.0°
$\mu = 1.58$ mm^{-1}
$T = 298$ (2) K
Plate, colorless
0.50 × 0.46 × 0.11 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
Absorption correction: ψ scan (*XCAD4*; Harms & Wocadlo, 1995)
$T_{min} = 0.458$, $T_{max} = 0.850$
1723 measured reflections
1587 independent reflections

1372 reflections with $I > 2\sigma(I)$
$R_{int} = 0.051$
$\theta_{max} = 26.0°$
$h = -8 \rightarrow 0$
$k = 0 \rightarrow 9$
$l = -37 \rightarrow 37$
3 standard reflections every 200 reflections intensity decay: 0.9%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.120$
$S = 1.12$
1587 reflections
122 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0961P)^2 + 4.1191P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.62$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn—O1	2.183 (2)	Zn—O4	1.981 (3)
Zn—O2	1.988 (2)		
O4—Zn—O2	127.17 (7)	O2^{i}—Zn—O1	88.65 (9)
O2^{i}—Zn—O2	105.65 (13)	O2—Zn—O1	92.41 (9)
O4—Zn—O1	89.12 (6)	O1—Zn—O1^{i}	178.24 (11)

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

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O1—H1A⋯O2^{ii}	0.85	1.93	2.772 (3)	170
O1—H1B⋯O6^{iii}	0.85	1.93	2.744 (4)	161
N1—H3⋯O6	0.86	2.15	2.913 (4)	148
O4—H4⋯O1^{ii}	0.84 (2)	1.95 (2)	2.771 (3)	165 (3)
O6—H6A⋯O5^{iv}	0.85	1.91	2.747 (3)	167
O6—H6B⋯O3^{v}	0.85	1.97	2.738 (3)	149

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

H atoms of the O1 and O6 water molecules were located in a difference Fourier map, idealized, and refined as riding, with O—H = 0.85 Å. Atom H4 was located in a difference Fourier map and refined subject to an O—H restraint of 0.85 (3) Å and an H⋯H restraint of 1.385 (3) Å. Other H atoms were placed at calculated positions, with C—H = 0.93 Å (aromatic) and 0.97 Å (methylene), and N—H = 0.86 Å, and refined using a riding model. In all cases, the U_{iso}(H) value is 1.2 times U_{eq} of the parent atom.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

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References

Burrows, A. D., Donovan, A. S., Harrington, R. W. & Mahon, M. (2004). *Eur. J. Inorg. Chem.* pp. 4686–4695.

Eddaoudi, M., Moler, D. B., Li, H., Chen, B., Reineke, T. M., O'Keeffe, M. & Yaghi, O. M. (2001). *Acc. Chem. Res.* **34**, 319–330.

Enraf–Nonius (1989). *CAD-4 Software*. Enraf-Nonius, Delft, The Netherlands.

Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.

James, S. (2003). *Chem. Soc. Rev.* **32**, 276–288.

Janiak, C. (2000). *J. Chem. Soc. Dalton Trans.* pp. 3885–3896.

Janiak, C. (2003). *J. Chem. Soc. Dalton Trans.* pp. 2781–2804.

Li, J.-R., Bu, X.-H. & Zhang, R.-H. (2004). *J. Chem. Soc. Dalton Trans.* pp. 813–819.

Manoj, N. & Vijayan, M. (2000). *J. Peptide Res.* **56**, 210–217.

Moulton, B. & Zaworotko, M. J. (2001). *Chem. Rev.* **101**, 1629–1658.

O'Keeffe, M., Eddaoudi, M., Li, H., Reineke, T. M. & Yaghi, O. M. (2000). *J. Solid State Chem.* **152**, 3–20.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Sheldrick, G. M. (2000). *SHELXTL*. Version 6.1. Bruker AXS Inc., Madison, Wisconsin, USA.

Yuan, Y., Xiao, R., Gao, G., Su, X.-Y., Yu, H., You, J. & Xie, R.-G. (2002). *J. Chem. Res.* (*S*), pp. 267–269.