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Key indicators

Single-crystal X-ray study
 T = 293 K
 Mean $\sigma(C-C) = 0.005 \text{ \AA}$
 Disorder in solvent or counterion
 R factor = 0.043
 wR factor = 0.122
 Data-to-parameter ratio = 15.6

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

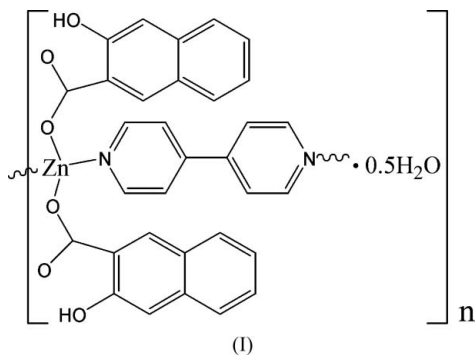
catena-Poly[[[bis(3-hydroxynaphthalene-2-carboxylato)zinc(II)]- μ -4,4'-bipyridine- $\kappa^2N:N'$] hemihydrate]

In the title complex, $[Zn(C_{11}H_7O_3)_2(C_{10}H_8N_2)] \cdot 0.5H_2O$, each Zn^{II} atom is coordinated by two N atoms from two 4,4'-bipyridine (bpy) ligands and two carboxylate O atoms from two 3-hydroxynaphthalene-2-carboxylate (hnc) ligands in a distorted tetrahedral geometry. The bpy ligands and Zn^{II} atoms form one-dimensional zigzag chains running along the c axis. The hnc ligands are located on both side of the chain. The chains are assembled into layers parallel to the bc plane, which are extended into a three-dimensional network by O—H...O hydrogen bonds and π – π stacking interactions.

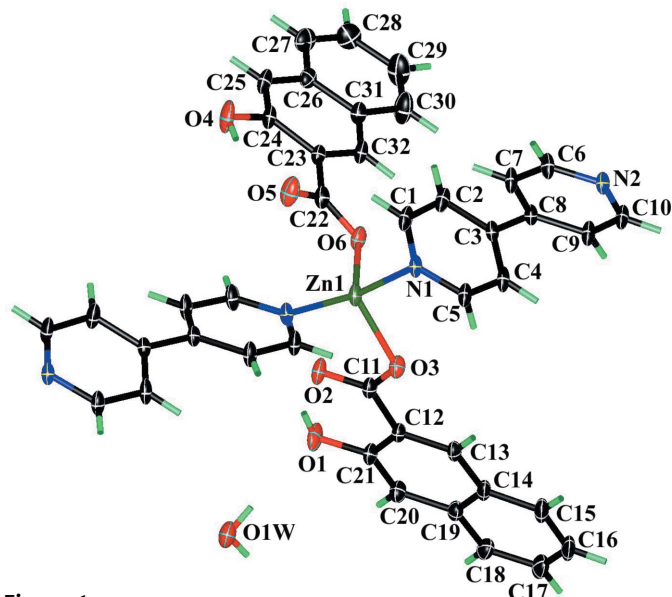
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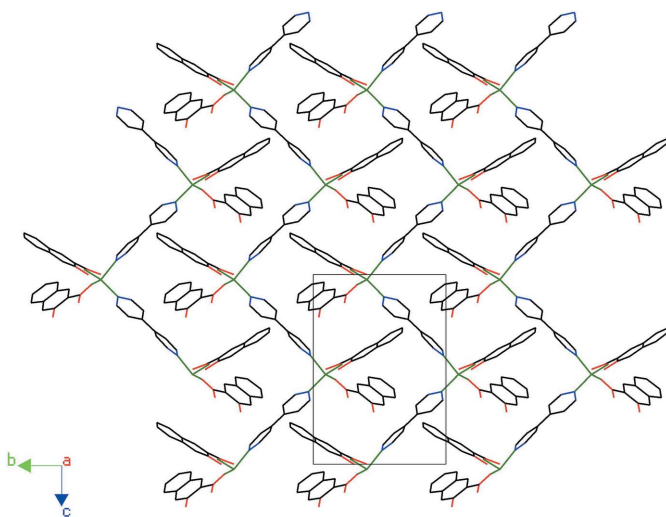
Supramolecular chemistry based on metal-ion-directed assembly of organic molecular building blocks is receiving extensive attention owing to their potential application in the fields of catalysis, non-linear optics, sensors, magnetism and molecular recognition (Lehn, 1995). Compared with simple inorganic compounds, coordination polymers hold great promise for their ease of processing, flexibility, structural diversity, and geometrical control, such as size, shape and symmetry. The principles of crystal engineering can be used to construct multi-dimensional frameworks in the solid state *via* supramolecular interactions (Plater *et al.*, 2000). In the construction of supramolecular frameworks, coordination polymers based on carboxylates and/or bipyridine-like ligands are of special interest. Many coordination polymers with interesting structures have been designed and synthesized (Eddaoudi *et al.*, 2002). Previous studies show that 2,2'-bipyridine-like chelate ligands give low-dimensional coordination polymers, especially one-dimensional chains with dicarboxylate ligands and transition metals under hydrothermal conditions (Sun *et al.*, 2003). We report here the crystal structure of the title complex, (I).



In complex (I), each Zn^{II} atom is coordinated by two N atoms from two chelating 4,4'-bipyridine (bpy) ligands and two carboxylate O atoms of two monodentate 3-hydroxy-

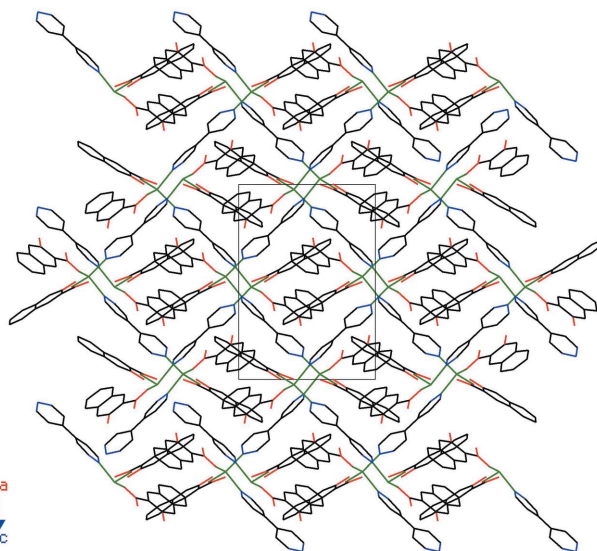

Figure 1

Part of the polymeric chain of (I), showing 50% probability displacement ellipsoids. Unlabelled atoms are related to labelled atoms by the symmetry operation $(x, \frac{5}{2} - y, \frac{1}{2} + z)$. The water molecule has a partial occupancy of 0.5.


Figure 2

A layer of zigzag chains of (I), viewed along the a axis. Water molecules and H atoms have been omitted for clarity.

naphthalene-2-carboxylate (hnc) ligands to furnish a distorted tetrahedral geometry (Fig. 1 and Table 1). The bpy ligands and Zn^{II} ions form one-dimensional zigzag chains, running along the c axis. The hnc ligands which are coordinated to the Zn^{II} atom are located on both side of the chain. These chains are further assembled into layers parallel to the bc plane via van der Waals interactions (Fig. 2), and the layers are extended into a three-dimensional network by aromatic π - π stacking interactions involving the bpy and hnc ligands (Fig. 3). The $Cg1 \cdots Cg2^i$, $Cg1 \cdots Cg3^i$, $Cg2 \cdots Cg3^{ii}$ and $Cg4 \cdots Cg4^{iii}$ distances are 3.820 (2), 3.830 (2), 3.791 (2) and 3.681 (2) Å, respectively; $Cg1$, $Cg2$, $Cg3$ and $Cg4$ are the centroids of the $N2/C6-C10$, $C12-C14/C19-C21$, $C14-C19$ and $C23-C26/C31/C32$ rings, respectively [symmetry codes: (i) $1 - x, 2 - y, 1 - z$; (ii) $1 - x, 1 - y, 1 - z$; (iii) $-x, 1 - y, 1 - z$]. The network structure is further stabilized by $O-H \cdots O$ hydrogen bonds involving the water molecules (Table 2).


Figure 3

The crystal packing of (I), viewed along the a axis. H atoms have been omitted for clarity.

$C32$ rings, respectively [symmetry codes: (i) $1 - x, 2 - y, 1 - z$; (ii) $1 - x, 1 - y, 1 - z$; (iii) $-x, 1 - y, 1 - z$]. The network structure is further stabilized by $O-H \cdots O$ hydrogen bonds involving the water molecules (Table 2).

Experimental

A mixture of $Zn(OAc)_2 \cdot 2H_2O$ (0.25 mmol), 4,4'-bipyridine (0.25 mmol), 3-hydroxy-naphthalene-2-carboxylic acid (0.5 mmol) and water (8 ml) was stirred for 15 min in air and then sealed in a Teflon reactor (23 ml). The reactor was heated at 443 K for 5 d and then cooled to room temperature at a rate of $5 K h^{-1}$. The resulting colourless block crystals were washed with deionized water and absolute ethanol (yield >30% based on Zn).

Crystal data

$[Zn(C_{11}H_7O_3)_2(C_{10}H_8N_2)] \cdot 0.5H_2O$
 $M_r = 604.89$
 Monoclinic, $P2_1/c$
 $a = 16.432$ (3) Å
 $b = 10.8059$ (17) Å
 $c = 16.627$ (3) Å
 $\beta = 112.100$ (3)°
 $V = 2735.4$ (8) Å³

$Z = 4$
 $D_x = 1.469 Mg m^{-3}$
 Mo $K\alpha$ radiation
 $\mu = 0.95 mm^{-1}$
 $T = 293$ (2) K
 Block, colourless
 $0.22 \times 0.20 \times 0.12 mm$

Data collection

Bruker SMART APEX area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2002)
 $T_{min} = 0.818$, $T_{max} = 0.895$

14832 measured reflections
 5906 independent reflections
 3942 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.028$
 $\theta_{max} = 27.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.122$
 $S = 1.01$
 5906 reflections
 379 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0578P)^2 + 0.8697P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} = 0.001$
 $\Delta\rho_{max} = 0.41 e \text{ \AA}^{-3}$
 $\Delta\rho_{min} = -0.23 e \text{ \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Zn1—O6	1.936 (2)	Zn1—N2 ⁱ	2.039 (2)
Zn1—O3	1.987 (2)	Zn1—N1	2.057 (2)
O6—Zn1—O3	108.78 (9)	O6—Zn1—N1	104.83 (9)
O6—Zn1—N2 ⁱ	128.04 (10)	O3—Zn1—N1	97.83 (9)
O3—Zn1—N2 ⁱ	111.58 (9)	N2 ⁱ —Zn1—N1	100.67 (9)

Symmetry code: (i) $x, -y + \frac{5}{2}, z + \frac{1}{2}$.

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1W—H1WA \cdots O3 ⁱⁱ	0.85	2.25	3.064 (7)	161
O1—H1A \cdots O2	0.82	1.80	2.533 (3)	149
O1W—H1WB \cdots O1	0.85	2.18	2.993 (7)	159
O4—h4A \cdots O5	0.82	1.86	2.586 (4)	147

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

The occupation factor of the water molecule was initially refined to 0.517 (8) and later fixed at 0.50. H atoms attached to O atoms were

located in a difference map and refined as riding on their parent atoms with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ (O—H = 0.82 and 0.85 Å). The C-bound H atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding on their parent C atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; 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*.

References

- Bruker (2000). *SHELXTL*. Version 6.12. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (2001). *SMART*. Version 5.625. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (2002). *SAINT* (Version 6.22) and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Eddaoudi, M., Kim, J., Rosi, N., Vodak, D., Wachter, J., O'Keeffe, M. & Yaghi, O. M. (2002). *Science*, **295**, 469–472.
- Lehn, J. M. (1995). *Supramolecular Chemistry*. Weinheim: VCH.
- Plater, M. J., Foreman, M. R. S. J., Gelbrich, T. & Hursthouse, M. B. (2000). *J. Chem. Soc. Dalton Trans.* pp. 1995–1996.
- Sun, X.-Z., Sun, Y.-F., Ye, B.-H. & Chen, X.-M. (2003). *Inorg. Chem. Commun.* **6**, 1412–1413.