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catena-Poly[[[(pyrazino[2,3-*f*][1,10]phenanthroline)zinc(II)]-μ-cyclohexane-1,4-dicarboxylato] dihydrate]

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Key indicators

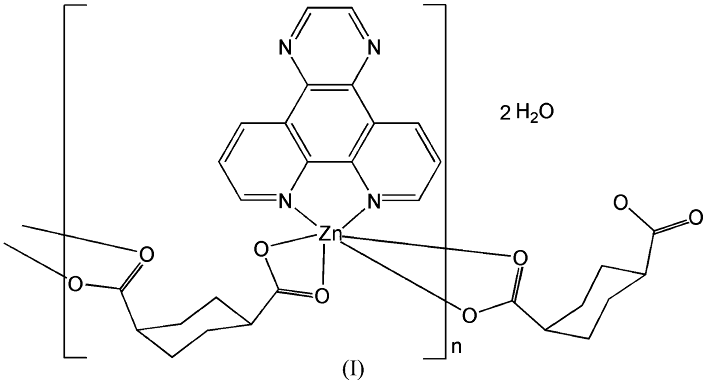
Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.005 Å
R factor = 0.051
wR factor = 0.146
Data-to-parameter ratio = 15.6

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

In the title compound, $\{[Zn(C_8H_{10}O_4)(C_{14}H_8N_4)]\cdot 2H_2O\}_n$ or [Zn(1,4-chdc)(PyPhen)]·$2H_2O$, where 1,4-chdc is the 1,4-cyclohexanedicarboxylate dianion and PyPhen is pyrazino[2,3-*f*][1,10]phenanthroline, the Zn^{II} atom is six-coordinated by one chelating PyPhen and two bidentate 1,4-chdc ligands, resulting in a distorted *cis*-ZnN_2O_4 octahedral geometry. The Zn^{II} centres are bridged by the 1,4-chdc ligands, forming an infinite one-dimensional helical chain. In addition, neighbouring chains interact through π–π interactions, generating a two-dimensional network.

Comment

Coordination polymers with helical structures have received much attention for their interesting structural features and potential application in optical devices, enantiomer separation, chiral synthesis and selective catalysis (Farrell *et al.*, 1995; Yaghi & Li, 1995).



(I)

We are now investigating the synthesis of coordination polymers based on divalent metals in combination with dicarboxylic acids and 1,10-phenanthroline (Phen) or its derivatives (Che, 2006). Cyclohexane-1,4-dicarboxylic acid (1,4-chdcH_2) possesses a flexible chair-type structure with *cis* and *trans* configurations for the attached carboxylic acid groups. Pyrazino[2,3-*f*][1,10]phenanthroline (PyPhen) is an important derivative of Phen that has been used to recognize the secondary structure of DNA in Ru^{II} complexes (Wu *et al.*, 1997). However, coordination polymers based on PyPhen in combination with flexible dicarboxylate ligands such as 1,4-chdc have rarely been studied. We report here the crystal structure of the title compound, (I) (Table 1).

In compound (I), the Zn^{II} centre is coordinated by four O atoms from two bidentate 1,4-chdc ligands and two N atoms from one PyPhen ligand in a distorted octahedral geometry (Fig. 1). The average Zn—O [2.160 (3) Å] and Zn—N

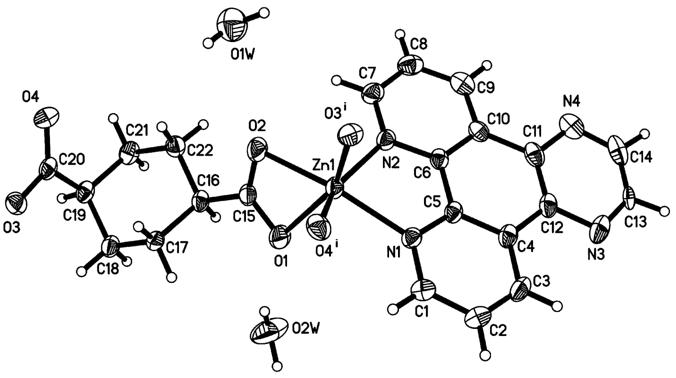


Figure 1
View of (I), showing the local coordination of the metal atom. Displacement ellipsoids are drawn at the 30% probability level (arbitrary spheres for the H atoms). [Symmetry code: (i) $2 - x, \frac{1}{2} + y, \frac{3}{2} - z$.]

distances [2.121 (3) Å] in (I) are comparable with those observed in $[Zn(tda)(phen)]_2 \cdot 5H_2O$ [tda = $S(CH_2COO)_2^{2-}$] (Grirrane *et al.*, 2006). Neighbouring Zn^{II} atoms are bridged by 1,4-chdc ligands, forming a one-dimensional single-chain structure (Fig. 2). The C—O bond lengths of both the 1,4-chdc carboxylate groups suggest that their bonding is essentially localized.

Neighbouring single chains are connected by π–π interactions, generating a two-dimensional supramolecular structure (Fig. 3). The π–π stacking distance (centroid separation) between PyPhen ligands in adjacent chains is 3.58 Å. In addition, there are hydrogen-bonding interactions between the uncoordinated water molecules and the 1,4-chdc carboxylate O atoms (Table 2). It is obvious that both π–π and hydrogen-bonding interactions help to improve the stability of current architectures (Noveron *et al.*, 2002).

Experimental

PyPhen was synthesized by the literature method (Dickeson & Summers, 1970). An ethanolic solution (10 ml) of PyPhen (0.5 mmol) was added slowly to an aqueous solution (10 ml) of $ZnCl_2 \cdot 2H_2O$ (0.5 mmol) and 1,4-chdcH_2 (1 mmol) with stirring at 353 K. The resulting solution was filtered and the filtrate was allowed to stand in air at room temperature for one week, yielding colourless crystals of (I) (75% yield based on Zn).

Crystal data

$[Zn(C_8H_{10}O_4)(C_{14}H_8N_4)] \cdot 2H_2O$
$M_r = 503.81$
Monoclinic, $P2_1/n$
$a = 8.1707 (16)$ Å
$b = 15.052 (3)$ Å
$c = 17.136 (3)$ Å
$\beta = 90.02 (3)°$
$V = 2107.5 (7)$ Å^3
$Z = 4$
$D_x = 1.588$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.22$ mm^{-1}
$T = 292 (2)$ K
Block, colourless
0.31 × 0.22 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.67$, $T_{max} = 0.80$
20456 measured reflections
4837 independent reflections
3641 reflections with $I > 2\sigma(I)$
$R_{int} = 0.044$
$\theta_{max} = 27.5°$

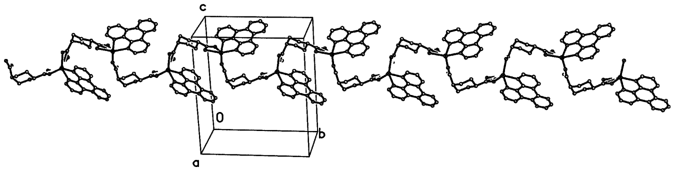


Figure 2
View of the chain structure of (I). H atoms have been omitted.

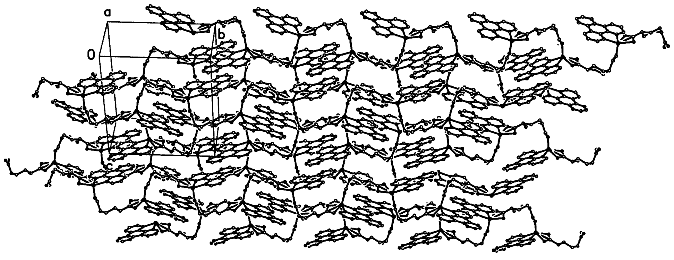


Figure 3
View of the two-dimensional supramolecular structure of (I) formed through the π–π interactions. H atoms have been omitted.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.146$
$S = 1.06$
4837 reflections
310 parameters
H-atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0708P)^2 + 2.0262P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.006$
$\Delta\rho_{max} = 0.77$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N1	2.110 (3)	Zn1—O4^i	2.321 (3)
Zn1—N2	2.132 (3)	C15—O2	1.236 (4)
Zn1—O1	2.096 (3)	C15—O1	1.271 (4)
Zn1—O2	2.167 (3)	C20—O4	1.234 (4)
Zn1—O3^i	2.056 (3)	C20—O3	1.284 (5)
N1—Zn1—N2	78.37 (11)	O3^i—Zn1—O4^i	59.19 (10)
O1—Zn1—O2	60.64 (10)		

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

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1W—HW12$\cdots$O2	0.86 (2)	2.42 (2)	3.019 (5)	128 (2)
O1W—HW11$\cdots$O2W^{ii}	0.94 (2)	1.97 (3)	2.788 (6)	145 (3)
O2W—HW22$\cdots$O1	0.90 (2)	1.99 (3)	2.768 (5)	144 (4)
O2W—HW21$\cdots$O3^{iii}	0.90 (4)	1.93 (4)	2.833 (5)	176 (4)

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

All H atoms on C atoms were positoned geometrically (C—H = 0.93 Å) and refined as riding atoms, with U_{iso}(H)= $1.2U_{eq}$(C). The H atoms of water molecules were located in difference Fourier maps and their positions were refined freely with a fixed U_{iso}(H) value of 0.059 Å^2.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*;

program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXTL-Plus*.

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References

Che, G.-B. (2006). *Acta Cryst.* E**62**, m1244–m1246.
Dickeson, J. E. & Summers, L. A. (1970). *Aust. J. Chem.* **23**, 1023–1027.
Farrell, R. P., Hambley, T. W. & Lay, P. A. (1995). *Inorg. Chem.* **34**, 757–758.
Grirrane, A., Pastor, A., A'lvarez, E., Mealli, C., Ienco, A. & Galindo, A. (2006). *Inorg. Chem. Commun.* **9**, 160–163.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Noveron, J. C., Lah, M. S., Sesto, R. E. D., Arif, A. M., Miller, J. S. & Stang, P. J. (2002). *J. Am. Chem. Soc.* **124**, 6613–6625.
Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (1990). *SHELXTL-Plus*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Góttingen, Germany.
Wu, J.-Z., Li, L., Zeng, T.-X., Ji, L.-N., Zhou, J.-Y., Luo, T. & Li, R.-H. (1997). *Polyhedron*, **16**, 103–107.
Yaghi, O. M. & Li, H. (1995). *J. Am. Chem. Soc.* **117**, 10401–10402.