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catena-Poly[[aqua(2,2′-bipyridine-*N*,*N*′)cadmium(II)]-*μ*-cyclohexane-1,4-dicarboxylato-$\kappa^4O,O':O'',O'''$] 2.5-hydrate]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean *σ*(C–C) = 0.003 Å
R factor = 0.023
wR factor = 0.054
Data-to-parameter ratio = 18.1

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

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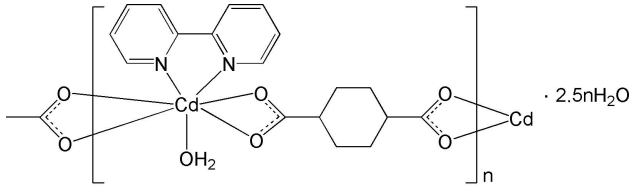
The title complex, $\{[Cd(C_8H_{10}O_4)(C_{10}H_8N_2)(H_2O)]\cdot 2.5H_2O\}_n$, shows a one-dimensional zigzag chain structure, in which the Cd atom is coordinated by two N atoms from a 2,2′-bipyridine ligand, a water molecule and four carboxylate O atoms from two different cyclohexane-1,4-dicarboxylate ligands.

Comment

In recent years, ligands containing carboxylate groups have been known to be good building blocks for the construction of polymeric structures (Wang *et al.*, 2006). Here we report a new coordination polymer, (I), constructed from the flexible ligand cyclohexane-1,4-dicarboxylate (chdc) and a Cd^{II} ion.



(I)

In the asymmetric unit of (I), there are one Cd^{II} atom, one chdc ligand, one 2,2′-bipyridine (2,2′-bpy), one coordinated water molecule and two and a half uncoordinated water

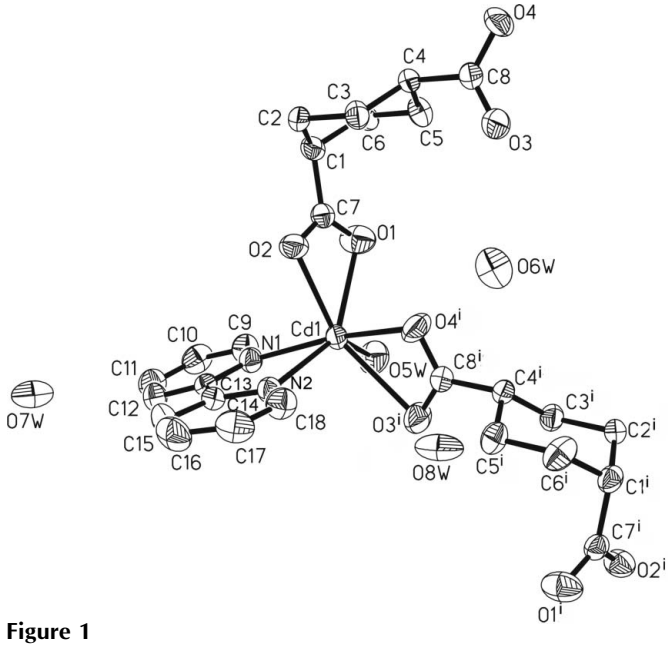


Figure 1
Part of the chain structure of (I). Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity. [Symmetry code: (i) $\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$.]

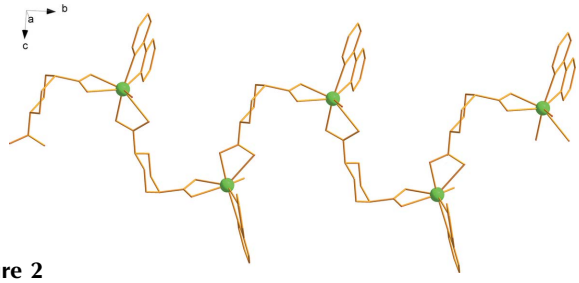


Figure 2
The one-dimensional zigzag chain in (I). H atoms and uncoordinated water molecules have been omitted for clarity.

molecules (Fig. 1). The Cd^{II} atom is seven-coordinated by four O atoms of two chelating carboxylate groups from two different chdc ligands, two N atoms from a 2,2′-bpy ligand and one water molecule. The chdc ligand connects the metal centers, forming an infinite zigzag chain along the *b* axis (Fig. 2). The 2,2′-bpy ligands decorate the chain on each side. The chains are linked to each other by hydrogen bonds between water molecules and carboxylate groups (Table 1). In the chdc ligand, the cyclohexane ring adopts a chair conformation. One carboxylate group lies in the *e*-bond position and the other in the *p*-bond position.

Experimental

$Cd(NO_3)_2{\cdot}4H_2O$ (0.062 g, 0.2 mmol), H_2chdc (0.035 g, 0.2 mmol) and 2,2′-bpy (0.031 g, 0.2 mmol) were dissolved in water (20 ml). To this solution, 1 *M* NaOH was added dropwise to give a pH of 6.0. The final solution was sealed in a 25 ml Teflon-lined stainless steel vessel, which was heated to 453 K for 3 d and then cooled to room temperature. Colorless prismatic crystals of (I) were collected (yield 42%).

Crystal data

$[Cd(C_8H_{10}O_4)(C_{10}H_8N_2)(H_2O)]{\cdot}2.5H_2O$
M_r = 501.81
Monoclinic, $C2/c$
a = 15.657 (2) Å
b = 13.140 (2) Å
c = 21.287 (3) Å
β = 111.129 (7)°
V = 4085.2 (11) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.11 mm^{-1}
T = 293 (2) K
0.35 × 0.25 × 0.15 mm

Data collection

Rigaku Mercury70 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.789, T_{max} = 0.893
(expected range = 0.748–0.846)
16648 measured reflections
4681 independent reflections
4397 reflections with $I > 2\sigma(I)$
R_{int} = 0.013

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.054
S = 1.07
4681 reflections
258 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O5*W*—H5*WA*···O8*W*	0.85	1.93	2.763 (3)	168
O5*W*—H5*WB*···O6*W*^{i}	0.85	2.02	2.797 (3)	152
O6*W*—H6*WA*···O1	0.85	2.44	3.251 (3)	159
O6*W*—H6*WB*···O1^{i}	0.85	2.00	2.770 (2)	150
O7*W*—H7*WA*···O4^{ii}	0.85	1.88	2.728 (2)	174
O7*W*—H7*WB*···O3^{iii}	0.85	1.95	2.760 (2)	159
O8*W*—H8*WA*···O7*W*^{iv}	0.85	1.84	2.629 (2)	153

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

All H atoms on C atoms were positioned geometrically and refined as riding, with C—H = 0.95 (aromatic ring), 0.99 (CH_2) or 1.00 Å (CH) and U_{iso}(H) = 1.2U_{eq}(C). H atoms on water molecules were located in a difference Fourier map and refined as riding (O—H = 0.85 Å), with U_{iso}(H) = 1.2U_{eq}(O).

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1994); software used to prepare material for publication: *SHELXTL*.

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References

Rigaku (2000). *CrystalClear*. Version 1.36. Rigaku MSC/SSI, Orem, Utah, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Siemens (1994). *SHELXTL*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Wang, J., Zheng, L. L., Li, G. J., Zheng, Y. Z. & Tong, M. L. (2006). *Cryst. Growth Des.* **6**, 357–359.