metal-organic papers

catena-Poly[[triaquacadmium(II)]-*μ*₂-pyrazine-2,3-dicarboxylato]

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The title Cd^{II} coordination polymer, $[Cd(C_6H_2N_2O_4)(H_2O)_3]_n$, was synthesized by reacting $Cd(NO_3)_2 \cdot 3H_2O$ and pyrazine-2,3-dicarboxylic acid under hydrothermal conditions. Single-crystal X-ray studies reveal that self-assembly between the bridging ligands and metal ions results in a one-dimensional coordination polymer, in which the Cd^{II} ion is hepta-coordinated and shows a $[CdNO_6]$ pentagonal–bipyramidal geometry.

Comment

Pyrazine-2,3-dicarboxylic acid ($pzdcH_2$) is a suitable multi-dentate bridging ligand to build polymeric coordination compounds. Up to now, the pzdc ligand and some simple d-block metal complexes have been X-ray characterized (Premkumar *et al.*, 2004; O'Connor *et al.*, 1982; Zou *et al.*, 1999). To our knowledge, no chiral coordination compounds assembled using the pzdc ligand and metal ions have been reported. Here we report the reaction of $pzdcH_2$ with a Cd^{II} salt, which afforded a chiral one-dimensional Cd^{II} coordination polymer, (I).

(I)
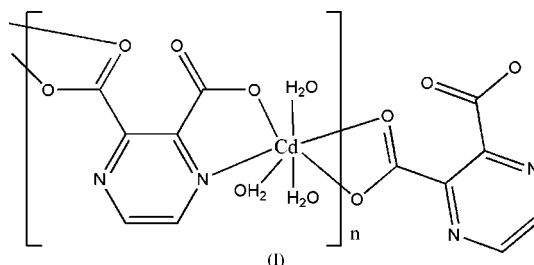
Complex (I) adopts a one-dimensional zigzag chain structure composed of Cd^{II} ions bridged by pzdc ligands (Fig. 1). One part of the ligand coordinates *via* N and O atoms, while the second carboxylate group contributes two O atoms to chelate the adjacent Cd^{II} ion. Corresponding bond lengths range from 2.287 (5) to 2.398 (5) Å (Table 1). Distorted pentagonal bipyramidal coordination around the metal centre is completed by three water molecules, with Cd—O bond lengths in the range 2.210 (5)–2.530 (5) Å. The zigzag chains are interconnected by an extensive network of hydrogen bonds operating *via* the coordinated water molecules, O atoms of carboxylate groups and N atoms of pzdc ligands, forming a three-dimensional framework (Fig. 2 and Table 2).

Experimental

A mixture of $Cd(NO_3)_2 \cdot 3H_2O$ (0.145 g, 0.5 mmol), pyrazine-2,3-dicarboxylic acid (0.084 g, 0.5 mmol), NaOH (0.04 g, 1 mmol) and

water (10 ml) was sealed in a 23 ml Teflon-lined reactor, heated at 453 K for 3 d, and then cooled to room temperature at a rate of 5 K h^{-1} (yield 20%). Analysis calculated for $C_6H_8CdN_2O_7$: C 21.67, H 2.42, N 8.42%; found: C 21.55, H 2.45, N 8.73%.

Crystal data

$[Cd(C_6H_2N_2O_4)(H_2O)_3]$	$Z = 4$
$M_r = 332.54$	$D_x = 2.299$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 5.7365$ (12) Å	$\mu = 2.30$ mm^{-1}
$b = 10.903$ (3) Å	$T = 293$ (2) K
$c = 15.362$ (3) Å	Block, colourless
$V = 960.8$ (3) Å^3	$0.37 \times 0.35 \times 0.27$ mm

Data collection

Bruker P4 diffractometer	1510 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.026$
Absorption correction: ψ scan (North et al., 1968)	$\theta_{max} = 27.5°$
$T_{min} = 0.450$, $T_{max} = 0.537$	3 standard reflections every 97 reflections
1798 measured reflections	intensity decay: <1%
1635 independent reflections	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.059P)^2 + 0.0261P]$
$R[F^2 > 2\sigma(F^2)] = 0.034$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.090$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.02$	$\Delta\rho_{max} = 1.30$ e Å^{-3}
1635 reflections	$\Delta\rho_{min} = -0.78$ e Å^{-3}
163 parameters	Absolute structure: Flack (1983), 331 Friedel pairs
H atoms treated by a mixture of independent and constrained refinement	Flack parameter: −0.06 (6)

Table 1
Selected geometric parameters (Å, °).

Cd1—O1^i	2.398 (5)	Cd1—O1W	2.530 (5)
Cd1—O2^i	2.398 (5)	Cd1—O2W	2.210 (5)
Cd1—O4	2.287 (5)	Cd1—O3W	2.387 (5)
Cd1—N2	2.346 (5)		
O2W—Cd1—O4	176.4 (3)	N2—Cd1—O3W	78.34 (19)
O2W—Cd1—N2	104.8 (3)	O4—Cd1—O1^i	85.37 (17)
O4—Cd1—N2	71.79 (17)	O4—Cd1—O2^i	88.69 (18)
O2W—Cd1—O3W	85.5 (2)	O1^i—Cd1—O2^i	54.82 (15)
O4—Cd1—O3W	94.9 (2)		

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

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1W—H1WB$\cdots$N1^{ii}	0.85 (2)	2.22 (5)	2.981 (7)	148 (8)
O1W—H1WA$\cdots$O4^{iii}	0.85 (2)	1.98 (4)	2.796 (7)	160 (8)
O2W—H2WA$\cdots$O2^{ii}	0.85 (2)	1.86 (3)	2.701 (8)	171 (13)
O2W—H2WB$\cdots$O2^{iv}	0.84 (2)	2.20 (8)	2.882 (8)	137 (11)
O2W—H2WB$\cdots$O3^{iv}	0.84 (2)	2.41 (8)	3.042 (9)	132 (9)
O3W—H3WA$\cdots$O1W^{iv}	0.85 (2)	2.12 (4)	2.916 (7)	157 (8)
O3W—H3WB$\cdots$O3^v	0.85 (2)	1.98 (6)	2.752 (8)	150 (10)

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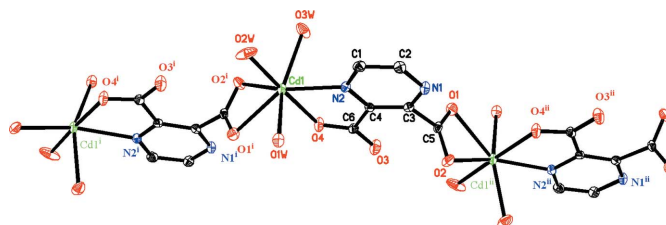

Figure 1
View of the structure of (I). Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity. Symmetry codes: (i) $-x + \frac{1}{2}, -y, z - \frac{1}{2}$; (ii) $-x + \frac{1}{2}, -y, z + \frac{1}{2}$.
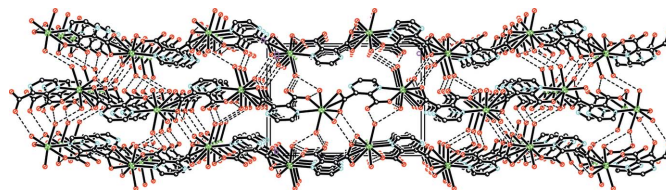

Figure 2
Plot depicting the hydrogen-bonded three-dimensional framework (dashed bonds) in the crystal structure of (I), as viewed down the [100] axis.

The water H atoms were located in a difference Fourier map and refined with free coordinates and an isotropic displacement parameter fixed at $U_{iso}(H) = 1.5U_{eq}(O)$. The geometry was regularized using restraints for distances O—H = 0.85 (2) Å and H$\cdots$H = 1.39 (1) Å. Other H atoms were placed in calculated positions and refined as riding on their carrier C atoms [C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$]. The highest peak is located 0.96 Å from atom Cd1.

Data collection: *XSCANS* (Bruker, 2001); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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