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A one-dimensional Cd^{II} coordination polymer: poly[[[bis[methanolcadmium(II)]-μ_2-aqua]-bis-(μ_3-pyridine-2,6-dicarboxylato-$\kappa^5O{:}O,N,O'{:}O'$)]

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.019
wR factor = 0.048
Data-to-parameter ratio = 12.6

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

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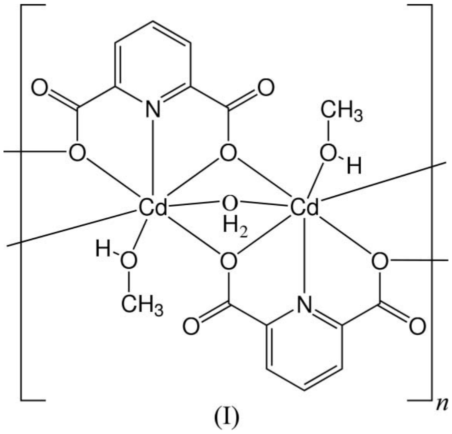
In the title complex, $[Cd_2(C_7H_3NO_4)_2(CH_3OH)_2(H_2O)]_n$, each Cd atom has a pentagonal–bipyramidal geometry ($CdNO_6$). The anionic pyridine-2,6-dicarboxylate (pydc) ligands adopt a $\kappa^5O{:}O,N,O'{:}O'$ coordination mode. Two symmetry-related Cd^{II} centers are linked by a pair of carboxylate groups from two pydc ligands as well as a bridging oxygen from a water molecule located on a twofold axis, to form a dinuclear unit. These dinuclear units are further connected *via* carboxylate O atoms to build a one-dimensional polymeric chain. O—H···O hydrogen bonds are observed within this chain.

Comment

Pyridine-2,6-dicarboxylic acid (H_2pydc) is a good chelating reagent with limited steric hindrance, and hitherto a large number of coordination complexes with this ligand have been studied (Sukanya *et al.*, 2006; Okabe & Oya, 2000*a*,*b*). In the case of Cd^{II} complexes, similar dinuclear structures are generally formed, in which the metal ions are bridged by the deprotonated ligand pydc (Odoko *et al.*, 2002) or its mono-ester derivative (Yang *et al.*, 2004) in the $\kappa^4O,N,O'{:}O$ coordination mode. In this context, we have recently prepared a new Cd^{II} complex with pyridine-2,6-dicarboxylic acid under normal conditions, namely $[Cd_2(\mu\text{-pydc})_2(\mu\text{-}H_2O)(CH_3OH)_2]_n$, (I).



(I)

In the structure of (I), all atoms are in general positions with the exception of the water molecule which is on a twofold axis. Each Cd^{II} center is seven-coordinated by four carboxylate O atoms and one pyridyl N atom from three pydc ligands, one O atom from methanol and the O atom of the bridging water molecule (Fig. 1). The coordination environment of Cd^{II} could be described as a pentagonal bipyramid in which the axial positions are occupied by two O atoms from carboxylate ($O1^{i}$)

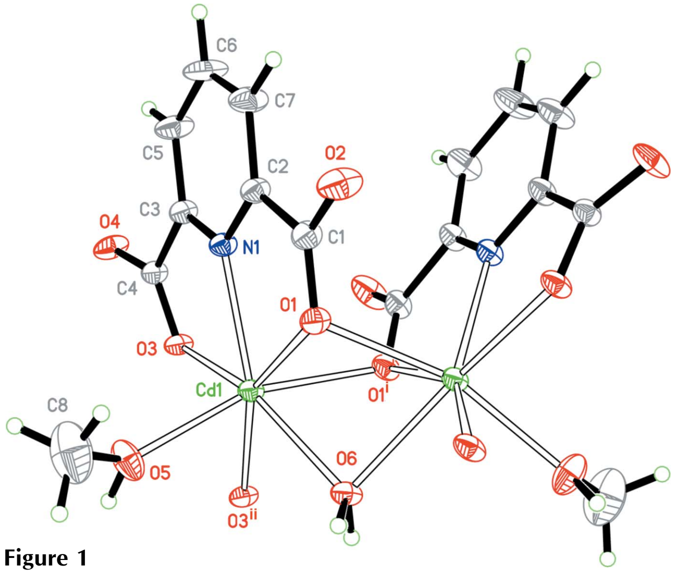


Figure 1
The dinuclear unit in the polymeric structure of (I) showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as spheres of arbitrary radii. [Symmetry code: (i) $-x, y, \frac{1}{2} - z$; (ii) $-x, -y, 1 - z$.]

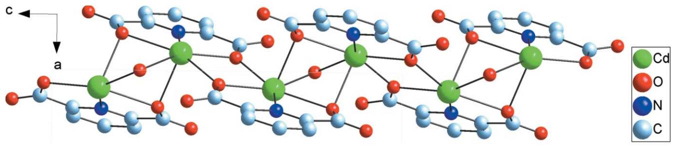


Figure 2
One-dimensional chain structure of (I) extending along the [001] direction. H atoms have been omitted for clarity.

and methanol (O5), respectively (symmetry codes as in Fig. 1). As depicted in Fig. 1, two adjacent Cd^{II} ions are joined by a pair of carboxylate O atoms (O1 and O1^i) from two pydc ligands to give a dinuclear unit with a Cd$\cdots$Cd separation of 3.4064 (5) Å. The occurrence of the bridging aqua ligand leads to a butterfly conformation for each Cd$_2$O$_2$ framework. The Cd—O1—Cd and Cd—O6—Cd bridging angles are 90.61 (6) and 91.18 (8)°, respectively. In this complex, each pydc ligand adopts the $\kappa^5 O{:}O,N,O'{:}O'$ binding mode, being different from that in the reported dinuclear Cd^{II}–pydc complexes (Odoko *et al.*, 2002; Yang *et al.*, 2004), and hence results in the formation of an extended polymeric structure. These dinuclear units are interconnected through bridging carboxylate O3 atoms to form a polymeric chain developing along [001] (Fig. 2). As a consequence, another Cd$_2$O$_2$ dinuclear core is formed with a planar conformation this time and a Cd$\cdots$Cd separation of 3.8303 (5) Å. The Cd—O3—Cd angle is 108.93 (7)°. All these structural features are similar to those of the dinuclear Cd^{II}–pydc species (Odoko *et al.*, 2002; Yang *et al.*, 2004). Furthermore, O—H$\cdots$O hydrogen bonds within the polymeric chains are observed (Table 1).

Experimental

A mixture of pyridine-2,6-dicarboxylic acid (8.4 mg, 0.05 mmol) and CdCl$_2$ (9.2 mg, 0.05 mmol) in methanol (10 ml) was stirred for 30 min at room temperature. The resulting clear solution was carefully layered over water (8 ml) in a straight test tube. Colorless block crystals suitable for X-ray diffraction were obtained after a period of 3 d (yield 6.3 mg, 40% based on H$_2$pydc).

Crystal data

[Cd$_2$(C$_7$H$_3$NO$_4$)$_2$(CH$_4$O)$_2$(H$_2$O)]
M_r = 637.11
Orthorhombic, *Pbcn*
a = 7.8099 (11) Å
b = 19.180 (3) Å
c = 13.4279 (18) Å
V = 2011.5 (5) Å^3
Z = 4
D_x = 2.104 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 2.18 mm^{-1}
T = 294 (2) K
Block, colorless
0.32 × 0.24 × 0.22 mm

Data collection

Bruker APEX-II CCD area-detector diffractometer
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{\min}$ = 0.578, $T_{\max}$ = 0.646
10139 measured reflections
1783 independent reflections
1507 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.023
$\theta_{\max}$ = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.019
$wR(F^2)$ = 0.048
S = 1.04
1783 reflections
142 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0231P)^2 + 1.659P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max}$ = 0.001
$\Delta\rho_{\max}$ = 0.26 e Å^{-3}
$\Delta\rho_{\min}$ = −0.52 e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O5—H5$A\cdots$O2^{iii}	0.93	1.79	2.684 (3)	161
O6—H6$A\cdots$O4^{ii}	0.95	1.70	2.604 (2)	159

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

The C-bound H atoms were positioned geometrically (C—H = 0.96 Å for methyl and 0.93 Å for pyridyl) and refined in the riding mode. The O-bound H atoms of methanol and water were first located in difference Fourier maps and then refined as riding with O—H distances of 0.93 and 0.95 Å, respectively. The $U_{\rm iso}$(H) values were set to 1.2 or 1.5 times $U_{\rm eq}$(parent atom).

Data collection: *APEXII* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001) and *DIAMOND* (Brandenburg, 2005); software used to prepare material for publication: *SHELXTL*.

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