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Poly[[μ_2-1,3-bis(pyridin-4-yl)propane]-(μ_3-1,4-phenylenediacetato)cadmium]

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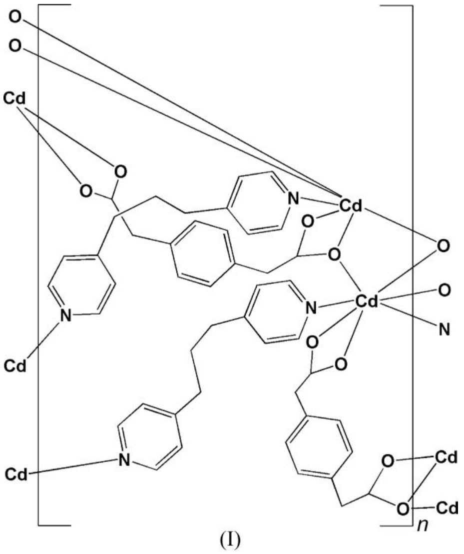
Solvothermal reaction between $Cd(NO_3)_2$, 1,4-phenylenediacetate (1,4-PDA) and 1,3-bis(pyridin-4-yl)propane (bpp) afforded the title complex, $[Cd(C_{10}H_8O_4)(C_{13}H_{14}N_2)]_n$. Adjacent carboxylate-bridged Cd^{II} ions are related by an inversion centre. The 1,4-PDA ligands adopt a *cis* conformation and connect the Cd^{II} ions to form a one-dimensional chain extending along the *c* axis. These chains are in turn linked into a two-dimensional network through bpp bridges. The bpp ligands adopt an *anti–gauche* conformation. From a topological point of view, each bpp ligand and each pair of 1,4-PDA ligands can be considered as linkers, while the dinuclear Cd^{II} unit can be regarded as a 6-connecting node. Thus, the structure can be simplified to a two-dimensional 6-connected network.

Comment

The design and construction of coordination polymers based on transition metals and organic spacers are currently attracting considerable attention (Moulton & Zaworotko, 2001; Kitagawa *et al.*, 2004). Flexible ligands such as 1,4-phenylenediacetate (1,4-PDA) and 1,3-bis(pyridin-4-yl)propane (bpp) are usually the typical building elements in coordination networks, since they can adopt varied coordination modes and geometries. For 1,4-PDA, the two carboxylate groups can exhibit various coordination modes. Furthermore, this flexible ligand can adopt either *cis* or *trans* conformations (Blake *et al.*, 2010; Lan *et al.*, 2011; Sposato *et al.*, 2010; Yang *et al.*, 2010). The bpp ligand is more flexible than 1,4-PDA due to its propyl group, and it can adopt *anti–anti*, *anti–gauche* or *gauche–gauche* conformations (Carlucci *et al.*, 2000; Hulvey *et al.*, 2010; Mao *et al.*, 1999). To understand further the coordination chemistry of flexible dicarboxylate and dipyridyl ligands, we employed these two ligands in a reaction with Cd^{II} ions under solvothermal conditions and obtained the title two-dimensional coordination polymer, $[Cd(C_{10}H_8O_4)(C_{13}H_{14}N_2)]_n$, (I).

As shown in Fig. 1, each Cd^{II} ion of (I) has a pentagonal–bipyramidal coordination, with five O atoms from three 1,4-PDA ligands occupying the equatorial sites and two N atoms from two bpp ligands located on the axial positions. The Cd—O bond lengths range from 2.313 (3) to 2.488 (3) Å, and the Cd—N distances are 2.340 (3) and 2.315 (3) Å. Two equivalent Cd^{II} ions related by an inversion centre with an interatomic distance of 3.7959 (9) Å are bridged by a single carboxylate O atom from each of two 1,4-PDA ligands to form a $[Cd_2(1,4\text{-PDA})_2]$ unit. Adjacent $[Cd_2(1,4\text{-PDA})_2]$ units are linked *via* a double bridge involving coordination at both ends of two 1,4-PDA ligands to afford a one-dimensional $[Cd_2(1,4\text{-PDA})_2]_n$ chain (Fig. 2). These chains are crosslinked through bridging bpp ligands to generate a rare two-dimensional 6-connected net. The size of each triangular grid in the two-dimensional net is 10.31 × 12.29 × 12.29 Å (Fig. 3).Different from that of the reported complex $\{[Cu_4(1,4\text{-PDA})_3(OH)_2(bpp)_2]2H_2O\}_n$ (Sposato *et al.*, 2010) constructed from *trans*-1,4-PDA and *anti–anti* bpp ligands, the conformations of the 1,4-PDA and bpp ligands in (I) are *cis–gauche* and *anti–gauche*, respectively.



(I)

The aromatic rings of the organic ligands of (I) are not close to one another. The closest ring–ring contact is between the N1/C1–C5 and $N2^i/C9^i–C13^i$ rings [symmetry code: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$], at a distance of 3.944 (3) Å.

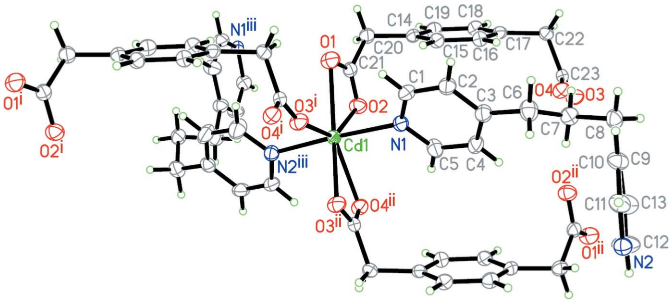


Figure 1
The coordination environment of the Cd^{II} ion in (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i) $x, y, z-1$; (ii) $-x+1, -y+1, -z$; (iii) $-x+1, y-\frac{1}{2}, -z-\frac{1}{2}$.]

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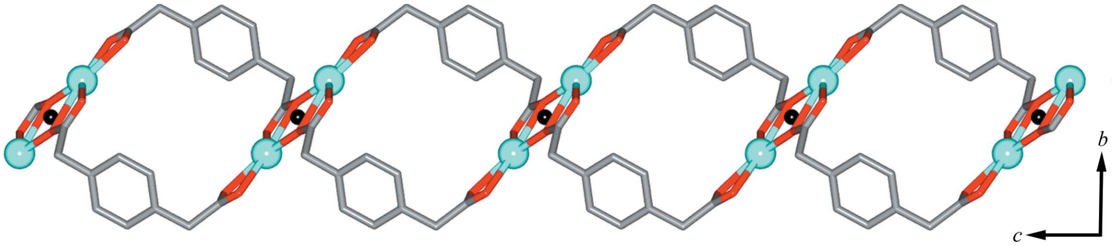

Figure 2
A view of the one-dimensional $[Cd(1,4\text{-PDA})]_n$ chain extending along the *c* axis. The black balls represent the inversion centres. The *a* axis is directed out of the paper towards the viewer.

Considering previously reported coordination polymers constructed from rigid dicarboxylate and dipyridyl ligands, we found that the structures of these complexes are usually two-dimensional (4,4) nets or three-dimensional frameworks. The structural motif of (I) is not only different from the reported rectangular sheets generated by metal ions and mixed ligands (Yang *et al.*, 2010), but also from the reported coordination polymers composed of three-dimensional networks (Tao *et al.*, 2000). The reason may be related to the flexibility of the 1,4-PDA ligand, which means the infinite $[Cd_2(1,4\text{-PDA})_2]_n$ chains cannot form a two-dimensional net. Furthermore, the flexibility of the bpp ligand also plays an important role in determining the final structure. In contrast with rigid dipyridyl ligands such as 4,4′-bipyridine (Liu *et al.*, 2009; Yang *et al.*, 2010), four flexible bpp ligands in (I) form bridges between four $[Cd_2(1,4\text{-PDA})_2]$ units and a central $[Cd_2(1,4\text{-PDA})_2]$ unit. These bridges complete links to two $[Cd_2(1,4\text{-PDA})_2]$ units in the $[Cd_2(1,4\text{-PDA})_2]_n$ chain on one side of the central unit and to a further two $[Cd_2(1,4\text{-PDA})_2]$ units in the chain on the other side of the central unit. Together with the intrachain links, these connections make each $[Cd_2(1,4\text{-PDA})_2]$ unit a 6-connecting node.

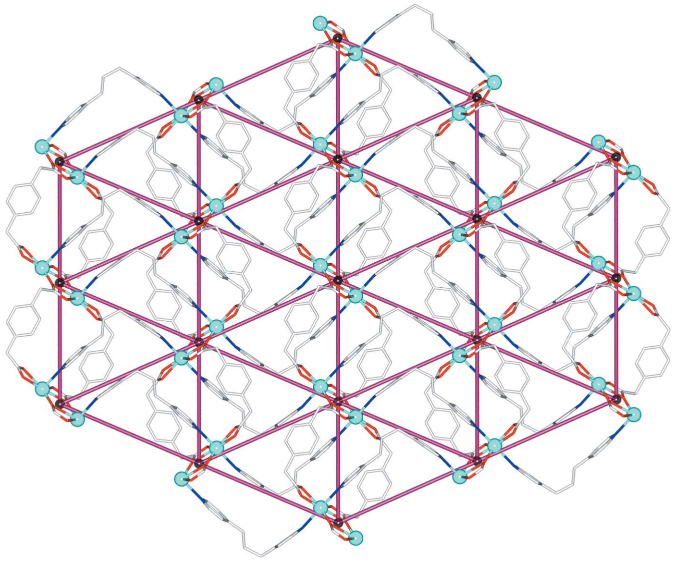

Figure 3
A view of the two-dimensional network of (I), extending along the *bc* axis. The black balls and thickest lines represent the topological net. The *a* axis is directed out of the paper towards the viewer.

In summary, a new two-dimensional coordination polymer, (I), constructed from flexible dicarboxylate and dipyridyl ligands has been presented. The structure is different from those constructed from mixed rigid ligands or a mixture of both rigid and flexible ligands. Thus, the flexibility of organic ligands plays an important role in constructing coordination networks. This work emphasizes the coordinative flexibility and versatility of mixed ligands and their synthetic utility in coordination chemistry. We are currently extending this study by preparing new ligands of this type with other substituted functional groups. We anticipate this approach to be useful for constructing novel coordination complexes.

Experimental

Into a 25 ml Teflon-lined stainless steel autoclave were loaded $Cd(NO_3)_2\cdot 4H_2O$ (154 mg, 0.5 mmol), 1,4-phenylenediacetic acid (97 mg, 0.5 mmol), 1,3-bis(pyridin-4-yl)propane (99 mg, 0.5 mmol), H_2O (8 ml) and EtOH (8 ml). The autoclave was sealed and heated in an oven to 433 K for 3 d, and then cooled to ambient temperature at a rate of 5 K h^{-1} to form colourless crystals of (I), which were washed with ethanol and dried in air (yield 188 mg, 75% based on Cd). Analysis calculated for $C_{23}H_{22}CdN_2O_4$: C 54.94, H 4.41, N 5.57%; found: C 54.62, H 4.18, N 5.75%. IR (KBr, ν, cm^{-1}): 1606 (*s*), 1590 (*s*), 1541 (*s*), 1506 (*m*), 1494 (*m*), 1401 (*s*), 1376 (*s*), 1226 (*m*), 1168 (*m*), 1069 (*m*), 1013 (*s*), 853 (*s*), 829 (*s*), 771 (*s*), 683 (*m*), 548 (*s*).

Crystal data

$[Cd(C_{10}H_8O_4)(C_{13}H_{14}N_2)]$
$M_r = 502.84$
Monoclinic, $P2_1/c$
$a = 10.022\ (2)$ Å
$b = 22.316\ (5)$ Å
$c = 10.316\ (2)$ Å
$\beta = 116.51\ (3)^\circ$
$V = 2064.6\ (9)$ Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 1.09$ mm^{-1}
$T = 223$ K
0.30 × 0.30 × 0.10 mm

Data collection

Rigaku Mercury CCD area-detector diffractometer
Absorption correction: multi-scan (*REQAB*; Jacobson, 1998)
$T_{min} = 0.736$, $T_{max} = 0.899$
11710 measured reflections
4699 independent reflections
3702 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.099$
$S = 1.10$
4699 reflections
271 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.60$ e Å^{-3}
$\Delta\rho_{min} = -0.53$ e Å^{-3}

All H atoms were placed in geometrically idealized positions, with C—H = 0.94 Å for phenyl and pyridyl groups or 0.98 Å for methylene groups, and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *CrystalClear* (Rigaku, 2001); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: QS3010). Services for accessing these data are described at the back of the journal.

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