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Poly[[(2,2′-bipyridine-κ²N:N′)cadmium(II)]-μ₃-5-hydroxyisophthalato-κ⁴O,O′:O″:O‴]

In the molecule of the title compound, $[Cd(C_8H_4O_5)(C_{10}H_8N_2)]_n$, the Cd atom is coordinated by two N and four O atoms of 2,2′-bipyridine and hydroxyisophthalate ligands, respectively, in a highly distorted octahedral geometry. 5-Hydroxyisophthalate acts as a tetradentate ligand, with one carboxylate group bidentate to one Cd atom and the other carboxylate group bidentate to two further Cd atoms, resulting in the formation of two-dimensional sheets.

Comment

The design and syntheses of supramolecular coordination polymer networks, especially those constructed via hydrogen bonding and π–π stacking interactions, has been a field of rapid growth because of their fascinating structures and promising applications in functional materials (Barton et al., 1999; Chen et al., 2005; Biradha et al., 2000). The coordination chemistry of aromatic polycarboxylate transition metal complexes has received considerable attention due to the variety of bridging modes of polycarboxylates in the formation of porous frameworks (Mori et al., 1997; Chui et al., 1999; Lo et al., 2000).

(I)
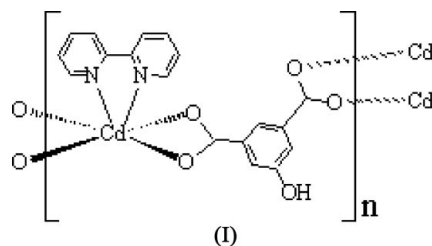
Encouraged by our successful synthesis of coordination polymers using transition metals, 3-sulfobenzoic acid and 2,2′-bipyridine (Li et al., 2005), we investigated the effect of replacing 3-sulfobenzoic acid with 5-hydroxyisophthalic acid. 5-Hydroxyisophthalic acid, OH—H₂BDC, like benzene-1,3,5-tricarboxylic acid, has two carboxylic acid groups arranged meta to each other, but with a phenol hydroxy group meta to both. This phenol hydroxy group was intended as a mimic for the third carboxy group, which remains protonated in other reported layered polymers (Plater et al., 1999; Cao et al., 2004). The title complex, (I), was obtained by the hydrothermal reaction of OH—H₂BDC with cadmium acetate and 2,2′-bipyidine, as a colorless solid in 60% yield.

In (I), each Cd[II] cation has a six-coordinate environment consisting of four carboxylate O atoms from three 5-hydroxyisophthalate anions and two N atoms from a 2,2′-bipyridine molecule (Fig. 1). The geometry around the Cd[II] cation is distorted octahedral, with Cd—O and Cd—N distances in the ranges 2.2374 (18)–2.528 (2) and 2.334 (2)–
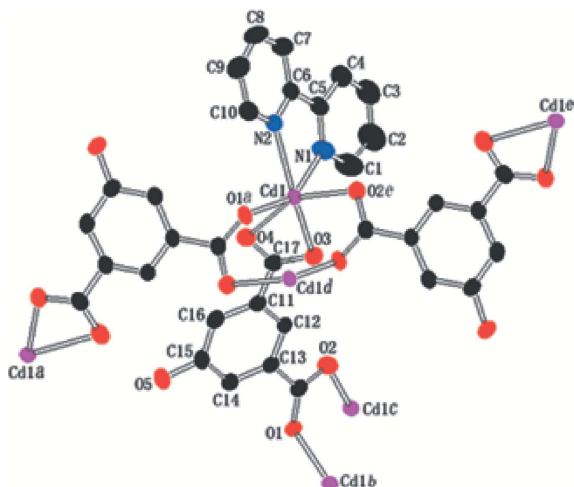
Figure 1
A segment of the structure with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity. [Symmetry codes: (a) $\frac{3}{2} - x$, $\frac{1}{2} + y$, $\frac{1}{2} - z$; (b) $\frac{1}{2} + x$, $\frac{3}{2} - y$, $\frac{1}{2} + z$; (c) $\frac{3}{2} - x$, $-\frac{1}{2} + y$, $\frac{1}{2} - z$; (d) $1 - x$, $2 - y$, $-z$; (e) $-\frac{1}{2} + x$, $\frac{3}{2} - y$, $-\frac{1}{2} + z$.]

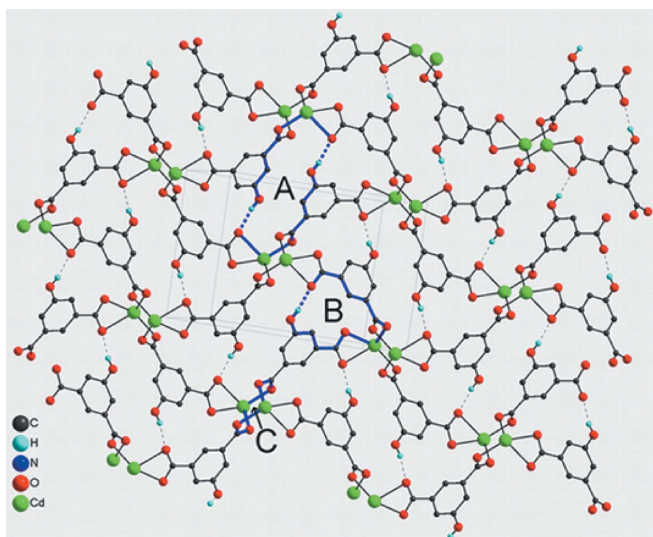**Figure 2**
A view of the title complex, showing how the organization of the three different subrings contribute to the construction of the $[Cd(OH-H_2BDC)]_n$ two-dimensional network. The three different subrings are labelled A, B and C.

2.370 (2) Å, respectively. The 2,2′-bipyridine ligand acts as a terminal ligand and the 5-hydroxyisophthalate anion functions as a tetradentate ligand, with one carboxylate group bidentate to one Cd atom and the other carboxylate bidentate to two further Cd atoms. As illustrated in Fig. 2, the OH–H₂BDC ligands link the cadmium centres in different ways to produce three different subrings.

The two-dimensional network of $[Cd(OH-H_2BDC)]_n$ units also contains an intermolecular O—H⋯O hydrogen bond (Table 2) and can be envisaged as being built up from interlocking 18-, 15- and 8-membered rings. The two-dimensional $[Cd(OH-H_2BDC)(2,2'-bipyridine)]_n$ layers are assembled into a three-dimensional framework via π–π stacking interactions.

Experimental

A mixture of CdSO₄ (0.021 g, 0.1 mmol), 5-hydroxyisophthalic acid (99%, 0.1 mmol), 2,2′-bipyridine (0.016 g, 0.1 mmol) and NaOH (0.008 g, 0.2 mmol) in H₂O (10 ml) was placed in a Parr Teflon-lined stainless steel vessel (23 ml), sealed and heated at 438 K for 3 d. The mixture was then cooled slowly to room temperature. Colourless crystals were obtained (yield 0.013 g, 60%, m.p. 503–504 K).

Crystal data

$[Cd(C_8H_4O_5)(C_{10}H_8N_2)]$	$D_x = 1.802$ Mg m^{-3}
$M_r = 448.71$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 3248
$a = 10.754$ (3) Å	reflections
$b = 10.073$ (2) Å	$\theta = 2.0–26.0°$
$c = 15.911$ (4) Å	$\mu = 1.35$ mm^{-1}
$\beta = 106.308$ (4)°	$T = 293$ (2) K
$V = 1654.2$ (7) Å^3	Block, colourless
$Z = 4$	$0.30 \times 0.25 \times 0.20$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer	3248 independent reflections
	2987 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.061$
Absorption correction: multi-scan (SADABS; Sheldrick, 2002a)	$\theta_{max} = 26.0°$
	$h = -10 \rightarrow 13$
$T_{min} = 0.67$, $T_{max} = 0.76$	$k = -11 \rightarrow 12$
7126 measured reflections	$l = -18 \rightarrow 19$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0433P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.028$	$+ 0.5583P]$
$wR(F^2) = 0.075$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.001$
3248 reflections	$\Delta\rho_{max} = 0.69$ e Å^{-3}
235 parameters	$\Delta\rho_{min} = -0.70$ e Å^{-3}
H-atom parameters constrained	Extinction correction: SHELXL
	Extinction coefficient: 0.003

Table 1
Selected geometric parameters (Å, °).

Cd1—O2^i	2.2374 (18)	Cd1—N1	2.370 (2)
Cd1—O4	2.2872 (18)	Cd1—O3	2.528 (2)
Cd1—O1^{ii}	2.3259 (18)	O1—Cd1^{iii}	2.3259 (18)
Cd1—N2	2.334 (2)	O2—Cd1^{iv}	2.2374 (18)
O2^i—Cd1—O4	151.08 (7)	O4—Cd1—O3	53.60 (6)
O2^i—Cd1—O1^{ii}	100.29 (7)	O1^{ii}—Cd1—O3	117.79 (6)
O4—Cd1—O1^{ii}	82.04 (6)	N2—Cd1—O3	148.23 (7)
O2^i—Cd1—N2	93.41 (7)	N1—Cd1—O3	82.40 (8)
O4—Cd1—N2	115.50 (7)	O2^i—Cd1—C17	126.51 (8)
O1^{ii}—Cd1—N2	85.92 (7)	O4—Cd1—C17	26.76 (7)
O2^i—Cd1—N1	90.71 (7)	O1^{ii}—Cd1—C17	98.64 (7)
O4—Cd1—N1	99.68 (8)	N2—Cd1—C17	137.57 (8)
O1^{ii}—Cd1—N1	153.81 (8)	N1—Cd1—C17	93.56 (8)
N2—Cd1—N1	69.63 (8)	O3—Cd1—C17	27.06 (7)
O2^i—Cd1—O3	101.94 (7)		

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

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O5—H5⋯O3^{ii}	0.82	1.88	2.677 (3)	165

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

H atoms were positioned geometrically, with O—H = 0.82 Å and C—H = 0.93 Å, and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C,O)$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2002*b*); software used to prepare material for publication: *SHELXTL*.

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