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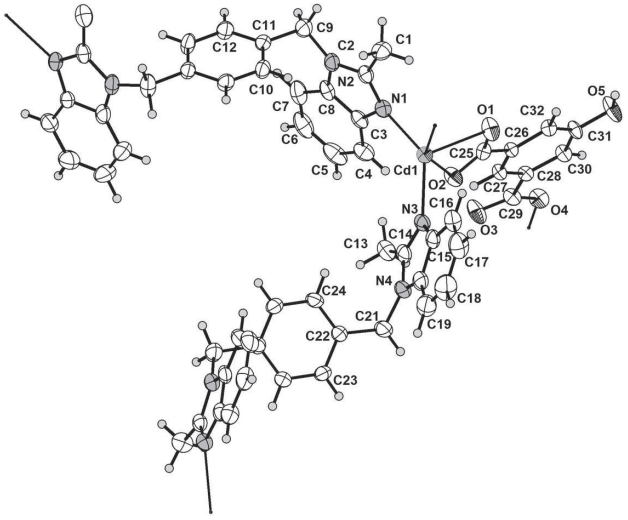
Crystal structure of *poly*-[μ-1,4-bis(2-ethylbenzimidazol-1-ylmethyl)benzene-κ²*N*:*N*′)-bis(μ₃-5-hydroxyisophthalate(2–)-κ³*O*,*O*′:*O*′′) dicadmium(II)] monohydrate, $C_{64}H_{54}N_8O_{11}Cd_2$



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Abstract

$C_{64}H_{54}Cd_2N_8O_{11}$, monoclinic, $P2_1/c$ (No. 14), $a = 10.314(2)$ Å, $b = 18.290(4)$ Å, $c = 16.516(6)$ Å, $\beta = 113.91(2)°$, $V = 2848.3(13)$ Å^3, $Z = 2$, $R_{gt}(F) = 0.0440$, $wR_{ref}(F^2) = 0.0890$, $T = 293(2)$K.

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Tables 1 and 2 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

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Table 1: Data collection and handling.

Crystal:	Colorless prism
	Size 0.32 × 0.26 × 0.22 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	8.2 cm^{-1}
Diffractometer, scan mode:	Rigaku Saturn 724, ω
$2\theta_{max}$, completeness:	58.2°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	18755, 5003, 0.043
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 4436
$N(param)_{refined}$:	395
Programs:	SHELX [7], CrystalClear [8]

Source of material

The title compound was prepared under the hydrothermal conditions. A mixture of 1,4-bis(2-methylbenzimidazol-1-ylmethyl)benzene (bmb) (73.2 mg, 0.2 mmol), $Cd(Ac)_2{\cdot}2H_2O$ (53.2 mg, 0.2 mmol), 5-hydroxyisophthalic acid (36.4 mg, 0.2 mmol), and H_2O (10 mL) were placed in a Teflon-lined stainless steel vessel, heated to 120 °C for 4 day, and then cooled to room temperature for 24 h. Colorless prism crystals of the title complex were obtained.

Experimental details

The structures were solved by direct methods and refined with the SHELX [7] software package. The hydrogen atoms were placed at calculated positions and refined as riding atoms with isotropic displacement parameters.

Discussion

Recent decades have seen increasing progress upon the design and syntheses of coordination polymers, not only due to their structures and new fascinating topologies, but also due to some potential applications, such as molecular recognition, heterogeneous catalysis, ion exchange, gas storage and separation, and chemical sensors [1–3]. However, to obtain desired structures of specific properties is still a challenge, because the self-assembly processes can be affected by many

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	x	y	z	U_{iso}*/U_{eq}
C1	0.2637(5)	0.9018(3)	0.1071(3)	0.0568(12)
H1A	0.1638	0.8920	0.0790	0.085*
H1B	0.2788	0.9497	0.1331	0.085*
H1C	0.3084	0.8660	0.1525	0.085*
C2	0.3259(4)	0.8980(2)	0.0403(2)	0.0406(9)
C3	0.4473(4)	0.8636(2)	−0.0345(2)	0.0419(10)
C4	0.5338(5)	0.8290(3)	−0.0684(3)	0.0542(12)
H4	0.5773	0.7846	−0.0453	0.065*
C5	0.5534(5)	0.8624(3)	−0.1377(3)	0.0690(15)
H5A	0.6100	0.8398	−0.1621	0.083*
C6	0.4907(6)	0.9288(3)	−0.1714(3)	0.0740(16)
H6	0.5072	0.9499	−0.2175	0.089*
C7	0.4046(5)	0.9645(3)	−0.1389(3)	0.0637(14)
H7	0.3621	1.0090	−0.1621	0.076*
C8	0.3844(4)	0.9305(2)	−0.0693(3)	0.0459(10)
C9	0.2191(5)	1.0155(2)	−0.0377(3)	0.0590(12)
H9A	0.2711	1.0572	−0.0454	0.071*
H9B	0.1975	1.0250	0.0132	0.071*
C10	0.0817(4)	1.0076(2)	−0.1192(3)	0.0433(10)
C11	−0.0049(4)	0.9468(2)	−0.1297(3)	0.0507(11)
H11	0.0220	0.9108	−0.0863	0.061*
C12	0.0382(4)	1.0597(2)	−0.1851(3)	0.0483(10)
H12	0.0942	1.1008	−0.1795	0.058*
C13	0.4484(5)	0.6301(3)	−0.0945(3)	0.0588(12)
H13A	0.4547	0.6808	−0.0781	0.088*
H13B	0.3948	0.6254	−0.1572	0.088*
H13C	0.5420	0.6108	−0.0788	0.088*
C14	0.3772(4)	0.5892(2)	−0.0473(3)	0.0460(10)
C15	0.2846(4)	0.5574(2)	0.0456(3)	0.0440(10)
C16	0.2398(5)	0.5524(3)	0.1141(3)	0.0571(12)
H16	0.2593	0.5891	0.1564	0.069*
C17	0.1647(6)	0.4903(3)	0.1165(4)	0.0774(16)
H17	0.1307	0.4855	0.1605	0.093*
C18	0.1391(6)	0.4345(3)	0.0537(4)	0.0859(19)
H18	0.0898	0.3931	0.0578	0.103*
C19	0.1836(5)	0.4387(3)	−0.0129(4)	0.0732(16)
H19	0.1650	0.4015	−0.0546	0.088*
C20	0.2582(4)	0.5008(2)	−0.0159(3)	0.0535(12)
C21	0.3116(5)	0.4810(3)	−0.1507(3)	0.0593(13)
H21A	0.3243	0.4294	−0.1359	0.071*
H21B	0.3884	0.4963	−0.1664	0.071*
C22	0.1718(4)	0.4915(2)	−0.2301(3)	0.0416(9)
C23	0.1299(4)	0.4395(2)	−0.2963(3)	0.0454(10)
H23	0.1870	0.3989	−0.2908	0.054*
C24	0.0871(4)	0.5519(2)	−0.2408(3)	0.0514(11)
H24	0.1146	0.5881	−0.1975	0.062*
C25	0.7016(4)	0.7319(2)	0.1701(3)	0.0339(8)
C26	0.8599(3)	0.73930(19)	0.2071(2)	0.0285(8)
C27	0.9270(4)	0.73397(19)	0.1494(2)	0.0318(8)
H27	0.8736	0.7293	0.0889	0.038*
C28	1.0738(4)	0.73562(19)	0.1823(2)	0.0306(8)
C29	1.1457(4)	0.7315(2)	0.1192(3)	0.0399(9)
C30	1.1520(4)	0.7418(2)	0.2723(2)	0.0360(9)
H30	1.2505	0.7408	0.2946	0.043*
C31	1.0853(4)	0.7496(2)	0.3300(2)	0.0369(9)
C32	0.9392(4)	0.74878(19)	0.2973(2)	0.0324(8)
H32	0.8939	0.7545	0.3355	0.039*
Cd1	0.41517(3)	0.727082(16)	0.082940(18)	0.03518(11)
N1	0.4077(3)	0.84411(18)	0.0342(2)	0.0402(8)
N2	0.3079(3)	0.95085(19)	−0.0208(2)	0.0452(8)
N3	0.3600(3)	0.61231(18)	0.0246(2)	0.0419(8)
N4	0.3198(4)	0.5219(2)	−0.0729(2)	0.0510(9)
O1	0.6348(3)	0.74288(18)	0.21688(18)	0.0525(8)
O2	0.6400(3)	0.71261(16)	0.08983(18)	0.0505(8)
O3	1.0714(3)	0.7318(2)	0.03852(18)	0.0633(9)
O4	1.2794(3)	0.72951(16)	0.15496(18)	0.0474(7)
O5	1.1694(3)	0.7586(2)	0.41760(18)	0.0659(10)
H5	1.1196	0.7655	0.4450	0.099*
O6[a]	0.5920(10)	0.8885(5)	0.2587(5)	0.104(3)
H61	0.67(2)	0.864(17)	0.29(2)	1.1(3)*

[a]Occupancy: 0.50.

factors, for instance, temperature, metal ions, ligands, metal-ligand ratios, solvents, and counterions [4–6].

As shown in the figure, the Cd(II) ion is five-coordinated in a trigonal bipyramid geometry, ligated by three oxygen atoms (O1, O2 and O4A) from two symmetry-related carboxylate groups of the 5-hydroxyisophthalate and two nitrogen atoms (N1 and N3A) from two bmb. The bond lengths are Cd(1)—O(1) = 2.459(3) Å, Cd(1)—O(2) = 2.291(2) Å, Cd(1)—O(4A) = 2.175(2) Å, Cd(1)—N(1) = 2.277(3) Å and Cd—N(3A) = 2.283(3) Å respectively. In the title complex, bmb adopts an asymmetric conformation with the $N_{donor}\cdots N—C_{sp3}\cdots C$ torsion of 117°. The two methylbenzimidazol arms of bmb bridge two adjacent Cd^{2+} ions to form a meso-helix chain in bidentate mode. The 1D Cd-bmb motif is linked by 5-hydroxyisophthalates to form 2D layers.

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