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The crystal structure of *catena*-poly[*diaqua*-(μ_4 -5-(benzo[*d*]thiazol-2-yl)benzene-1,3-dicarboxylate- $\kappa^4 O, O': O'', O'''$)-(μ_4 -5-(benzo[*d*]thiazol-2-yl)benzene-1,3-dicarboxylate- $\kappa^4 O, O': O'', O'''$)dicadmium(II)], $C_{30}H_{18}Cd_2N_2O_{10}S_2$

Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.24 × 0.22 × 0.21 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	1.74 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω -scans
$\theta_{\max}$, completeness:	28.5°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	64888, 6605, 0.039
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 5869
$N(\text{param})_{\text{refined}}$:	415
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 3]

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Abstract

$C_{30}H_{18}Cd_2N_2O_{10}S_2$, monoclinic, $P2_1/c$ (no. 14), $a = 14.9275(2)$ Å, $b = 10.18003(11)$ Å, $c = 18.3497(2)$ Å, $\beta = 92.0808(13)^\circ$, $V = 2786.63(6)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0285$, $wR_{\text{ref}}(F^2) = 0.0679$, $T = 290.3(9)$ K.

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The crystal structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of materials

A mixture of $Cd(CH_3COO)_2 \cdot 2H_2O$ (0.0266 g, 0.1 mmol), 5-(benzo[*d*]thiazol-2-yl)benzene-1,3-dioic acid (0.0299 g, 0.1 mmol), H_2O (10 mL) and ethanol (5 mL) was sealed in a 25 mL Teflon-lined stainless steel vessel and heated at 90 °C for 3 days. Yellow block crystals of the title compound were obtained, which were washed with water and dried in air with a 56% yield.

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	0.37333(2)	0.20899(2)	0.25690(2)	0.02403(6)
Cd2	0.49620(2)	0.94537(2)	0.35360(2)	0.02303(6)
S1	−0.00271(6)	0.56829(8)	0.10176(5)	0.0443(2)
S2	0.80776(6)	0.29197(8)	0.57628(5)	0.0465(2)
O1	0.40191(13)	0.45732(18)	0.23925(10)	0.0291(4)
O2	0.27234(14)	0.35913(18)	0.21599(12)	0.0379(5)
O3	0.38424(14)	0.9599(2)	0.26988(12)	0.0361(5)
O4	0.27524(16)	1.05775(18)	0.21109(15)	0.0478(6)
O5	0.48574(15)	0.2064(2)	0.34060(12)	0.0379(5)
O6	0.57321(14)	0.10085(17)	0.41887(10)	0.0306(4)
O7	0.55233(15)	0.79903(17)	0.44461(11)	0.0355(5)
O8	0.52349(13)	0.71365(17)	0.33623(10)	0.0289(4)
O9	0.28867(17)	0.2133(2)	0.36397(13)	0.0468(6)
H9A	0.2899	0.1376	0.3836	0.070*
H9B	0.2813	0.2933	0.3729	0.070*
O10	0.38421(15)	0.9863(2)	0.43807(12)	0.0437(5)
H10A	0.3699	0.9324	0.4743	0.066*
H10B	0.3904	1.0589	0.4578	0.066*
N1	0.03810(16)	0.8105(3)	0.06064(15)	0.0372(6)
N2	0.77486(17)	0.5328(2)	0.60902(13)	0.0310(5)
C1	0.27347(17)	0.5904(2)	0.20737(14)	0.0231(5)
C2	0.31295(17)	0.7076(2)	0.23000(14)	0.0225(5)
H2	0.3665	0.7072	0.2575	0.027*
C3	0.27119(17)	0.8265(2)	0.21096(14)	0.0222(5)
C4	0.19193(17)	0.8260(2)	0.16876(15)	0.0251(5)
H4	0.1659	0.9054	0.1545	0.030*
C5	0.15089(18)	0.7083(2)	0.14740(15)	0.0246(5)
C6	0.19237(18)	0.5912(2)	0.16802(15)	0.0253(5)
H6	0.1652	0.5119	0.1552	0.030*

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Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
C7	0.31859(19)	0.4612(2)	0.22186(14)	0.0252(6)
C8	0.31224(18)	0.9549(2)	0.23256(15)	0.0250(5)
C9	0.06657(18)	0.7081(2)	0.10307(15)	0.0261(6)
C10	−0.0435(2)	0.7717(3)	0.02639(17)	0.0361(7)
C11	−0.0745(2)	0.6473(3)	0.04180(17)	0.0363(7)
C12	−0.1549(2)	0.5998(4)	0.0079(2)	0.0502(9)
H12	−0.1771	0.5166	0.0180	0.060*
C13	−0.1988(2)	0.6836(4)	−0.04120(19)	0.0505(9)
H13	−0.2515	0.6556	−0.0649	0.061*
C14	−0.1665(3)	0.8062(4)	−0.0555(2)	0.0583(10)
H14	−0.1975	0.8590	−0.0892	0.070*
C15	−0.0905(3)	0.8533(4)	−0.0221(2)	0.0518(9)
H15	−0.0704	0.9379	−0.0314	0.062*
C16	0.57379(17)	0.3334(2)	0.42519(14)	0.0216(5)
C17	0.54385(18)	0.4546(2)	0.39845(14)	0.0223(5)
H17	0.5032	0.4587	0.3589	0.027*
C18	0.57552(18)	0.5697(2)	0.43177(14)	0.0224(5)
C19	0.63655(18)	0.5636(2)	0.49050(14)	0.0247(5)
H19	0.6554	0.6407	0.5136	0.030*
C20	0.66997(18)	0.4429(2)	0.51534(14)	0.0245(5)
C21	0.63729(18)	0.3291(2)	0.48217(14)	0.0247(5)
H21	0.6585	0.2481	0.4986	0.030*
C22	0.54160(19)	0.2065(2)	0.39277(15)	0.0249(5)
C23	0.54877(18)	0.7020(2)	0.40338(15)	0.0247(5)
C24	0.74465(19)	0.4358(2)	0.56945(15)	0.0277(6)
C25	0.8542(2)	0.4991(3)	0.64665(15)	0.0320(6)
C26	0.8830(2)	0.3704(3)	0.63475(17)	0.0381(7)
C27	0.9647(2)	0.3249(4)	0.6641(2)	0.0498(9)
H27	0.9839	0.2397	0.6553	0.060*
C28	1.0157(2)	0.4085(4)	0.7061(2)	0.0529(9)
H28	1.0705	0.3803	0.7260	0.064*
C29	0.9866(2)	0.5352(4)	0.71935(18)	0.0480(9)
H29	1.0225	0.5901	0.7485	0.058*
C30	0.9065(2)	0.5824(3)	0.69077(17)	0.0403(7)
H30	0.8879	0.6675	0.7006	0.048*

Experimental details

All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined as riding on their parent atoms with $U_{\text{iso}}(\text{H}) = 1.2$ times $U_{\text{eq}}(\text{C})$ and $U_{\text{iso}}(\text{H}) = 1.5$ times $U_{\text{eq}}(\text{O})$. There is some evidence of minor disorder in one of the two benzothiazole rings (S1, N1), which was not modelled during refinement.

Comment

Coordination polymer (CPs) have been extensively investigated in the past few decades because of their vast applications such as gas storage [4], catalysis [5], molecular magnetism [6], luminescence [7], and so on. In particular, luminescent CPs based on d¹⁰ metal ions and conjugated organic ligands have emerged as a rapidly growing field of research [8–10]. Among these, Cd(II) CPs are one of the most interesting luminescent CPs [11, 12]. It is well known that the properties of CPs mainly depend on the organic ligands

and the center metal ions because they are involved in the formation of the final CPs [13, 14]. This provides us with the opportunity to rationally select the precursors, which enables synthesis of CPs for specific structures and properties. Herein, we report a Cd(II) CPs based on a bifunctional ligand 5-(benzo[d]thiazol-2-yl)benzene-1,3-dioic acid. Other Cd(II)-based coordination polymers related to the title structure have been reported in the literature [15].

The title compound exhibits a one dimensional chain structure. The asymmetric unit of the title structure contains two Cd(II) ions, two 5-(benzo[d]thiazol-2-yl)benzene-1,3-dioic acid anions, and two coordinated water molecules. As shown in the figure, each metal atom is seven-coordinated by six oxygen atoms from four different 5-(benzo[d]thiazol-2-yl)benzene-1,3-dioic acid ligands and one oxygen atom from a water molecule; the coordination geometry can be described as a distorted pentagonal bipyramid. The Cd—O bond lengths are in the range of 2.233(2)–2.672(2) Å. Nitrogen atoms do not take part in the coordination. Four carboxylates adopt μ_2 - η^2 : η^1 or μ_2 - η^1 : η^1 modes (not shown in the figure), by which pairs of Cd(II) cations are connected into a one-dimensional chain structure along the *b*-axis. The one-dimensional chains are linked by several classical and non-classical hydrogen bonds to form a three-dimensional supramolecular structure.

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