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The crystal structure of *catena*-poly[(μ_2 -4-(benzo[d]imidazol-2-yl)benzenecarboxylato- $\kappa^2 N, O$)-(μ_2 -4-(benzo[d]imidazol-2-yl)benzenecarboxylato- $\kappa^3 N, O:O'$)cadmium(II)]dihydrate, $C_{28}H_{22}CdN_4O_6$

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.21 × 0.20 × 0.18 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.95 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω
$\theta_{\max}$, completeness:	28.4°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	14591, 5202, 0.033
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 4658
$N(\text{param})_{\text{refined}}$:	352
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 3]

<https://doi.org/10.1515/ncrs-2020-0149>

Received March 19, 2020; accepted June 2, 2020; available online July 14, 2020

Abstract

$C_{28}H_{22}CdN_4O_6$, triclinic, $P\bar{1}$ (no. 2), $a = 8.8463(3)$ Å, $b = 9.0275(3)$ Å, $c = 15.6752(5)$ Å, $\alpha = 78.033(3)^\circ$, $\beta = 88.988(3)^\circ$, $\gamma = 84.843(3)^\circ$, $V = 1219.66(7)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0333$, $wR_{\text{ref}}(F^2) = 0.0732$, $T = 291$ K.

CCDC no.: 2007141

A part of the polymeric structure is shown in the figure ($A = 1 - x$, $1 - y$, $1 - z$; $B = 2 - x$, $1 - y$, $-z$). Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

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

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	0.68235(2)	0.33201(2)	0.24244(2)	0.02708(8)
O1	0.5787(3)	0.5241(2)	0.29394(14)	0.0497(6)
O2	0.4117(2)	0.3628(3)	0.34559(16)	0.0509(6)
O3	1.0552(2)	0.6371(2)	−0.22212(13)	0.0427(5)
O4	1.2161(2)	0.4731(2)	−0.13856(13)	0.0367(5)
N1	0.1874(3)	1.0363(2)	0.52732(15)	0.0333(5)
H1	0.1746	1.0729	0.4725	0.040*
N2	0.2535(2)	0.8724(2)	0.64975(14)	0.0268(5)
N3	0.5776(2)	0.2362(2)	0.13622(14)	0.0271(5)
N4	0.4855(2)	0.2063(2)	0.01061(15)	0.0304(5)
H4	0.4764	0.2131	−0.0446	0.036*
C1	0.4072(3)	0.5927(3)	0.39922(17)	0.0294(6)
C2	0.4613(3)	0.7350(3)	0.38981(19)	0.0381(7)
H2	0.5338	0.7647	0.3475	0.046*
C3	0.4082(3)	0.8320(3)	0.44258(19)	0.0382(7)
H3	0.4418	0.9287	0.4339	0.046*
C4	0.3051(3)	0.7878(3)	0.50887(17)	0.0280(6)
C5	0.2548(3)	0.6439(3)	0.52011(19)	0.0333(6)
H5	0.1871	0.6117	0.5647	0.040*
C6	0.3050(3)	0.5482(3)	0.46520(19)	0.0336(6)
H6	0.2695	0.4524	0.4728	0.040*
C7	0.4669(3)	0.4847(3)	0.34235(19)	0.0362(7)
C8	0.2492(3)	0.8948(3)	0.56325(17)	0.0270(6)
C9	0.1488(3)	1.1112(3)	0.59319(18)	0.0289(6)
C10	0.0818(3)	1.2566(3)	0.5932(2)	0.0382(7)
H10	0.0519	1.3236	0.5416	0.046*
C11	0.0619(3)	1.2969(3)	0.6724(2)	0.0424(8)
H11	0.0160	1.3927	0.6749	0.051*
C12	0.1089(4)	1.1973(3)	0.7493(2)	0.0422(7)
H12	0.0970	1.2295	0.8018	0.051*
C13	0.1726(3)	1.0521(3)	0.74954(19)	0.0358(7)

Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
H13	0.2021	0.9856	0.8013	0.043*
C14	0.1914(3)	1.0087(3)	0.67009(17)	0.0273(6)
C15	0.9544(3)	0.4520(3)	−0.10898(17)	0.0273(6)
C16	0.8041(3)	0.4979(3)	−0.13176(19)	0.0345(7)
H16	0.7812	0.5704	−0.1823	0.041*
C17	0.6881(3)	0.4363(3)	−0.07966(19)	0.0343(7)
H17	0.5877	0.4663	−0.0960	0.041*
C18	0.7206(3)	0.3296(3)	−0.00280(17)	0.0271(6)
C19	0.8716(3)	0.2827(3)	0.01944(18)	0.0294(6)
H19	0.8950	0.2108	0.0702	0.035*
C20	0.9862(3)	0.3426(3)	−0.03363(18)	0.0297(6)
H20	1.0867	0.3093	−0.0188	0.036*
C21	1.0833(3)	0.5245(3)	−0.16039(18)	0.0315(6)
C22	0.5956(3)	0.2608(3)	0.04967(17)	0.0263(6)
C23	0.3900(3)	0.1381(3)	0.07347(18)	0.0294(6)
C24	0.2655(3)	0.0576(3)	0.0684(2)	0.0379(7)
H24	0.2299	0.0439	0.0154	0.045*
C25	0.1976(3)	−0.0009(4)	0.1459(2)	0.0463(8)
H25	0.1143	−0.0566	0.1454	0.056*
C26	0.2501(4)	0.0207(4)	0.2251(2)	0.0467(8)
H26	0.1993	−0.0187	0.2760	0.056*
C27	0.3753(3)	0.0990(3)	0.23027(19)	0.0372(7)
H27	0.4102	0.1124	0.2835	0.045*
C28	0.4473(3)	0.1572(3)	0.15250(18)	0.0277(6)
O5	0.1269(3)	1.2499(3)	0.37493(14)	0.0538(6)
H5A	0.0962	1.2645	0.3226	0.081*
H5B	0.2111	1.2884	0.3641	0.081*
O6	0.4477(3)	0.2081(3)	−0.16039(15)	0.0621(7)
H6A	0.3580	0.1708	−0.1462	0.093*
H6B	0.4354	0.2988	−0.1897	0.093*

Source of material

A mixture of Cd(CH₃COO)₂ · 2 H₂O (0.0266 g, 0.1 mmol), 4-(benzo[d]imidazol-2-yl)benzoic acid (0.0238 g, 0.1 mmol), and H₂O (15 mL) was sealed in a 25 mL Teflon-lined stainless steel vessel and heated at 120 °C for 4 days. The colorless block crystals of the title compound were obtained, which were washed with water and dried in air with a 44% yield.

Experimental details

The hydrogen atoms were assigned with common isotropic displacement factors $U_{\text{iso}}(\text{H}) = 1.2$ times $U_{\text{eq}}(\text{C})$ and $U_{\text{eq}}(\text{N})$, refined with riding coordinates, $U_{\text{iso}}(\text{H}) = 1.5$ times $U_{\text{eq}}(\text{O})$, refined as rotating group.

Comment

Coordination polymer (CPs), a fascinating kind of crystalline solids have drawn attention in the past decades because of their porosity, tunable frameworks, and application in many fields [4–7]. Up to now various techniques have been developed to build CPs due to the aesthetic appeal of their frameworks and topologies. A number of CPs have been assembled

from metal centers with aromatic carboxylates since they can provide the structural rigidity and give diverse coordination modes for the generation of CPs chains, layers, or networks [8–10]. On the other hand, N-donor coligands can be incorporated, thereby enhancing the structural scope and imparting additional multi-functional behavior [11–13]. Recently, we have been interested in the construction of CPs bearing bifunctional ligands with aromatic carboxylates and N-heterocyclics present together [14–16]. As an extension of this project, we herein report the title structure.

The title compound exhibits one dimensional chain structure. The asymmetric unit of the title structure contains two 4-(benzo[d]imidazol-2-yl)benzoate anions, one Cd(II) ion, and two lattice water molecules. As shown in the figure, Cd1 is five-coordinated by three oxygen atoms from two different 4-(benzo[d]imidazol-2-yl)benzoate ligands and two nitrogen atoms from two other ligands. The coordination geometry of Cd1 can be described as a distorted trigonal bipyramid. The Cd–O bond lengths are in the range of 2.183(2)–2.372(2) Å, and the Cd–N bond lengths are 2.266(2) and 2.275(2) Å, respectively. The two 4-(benzo[d]imidazol-2-yl)benzoate ligands adopt different μ_2 coordination modes and each Cd(II) center is coordinated by four ligands. Cd(II) cations are connected into one-dimensional chains. There are several intermolecular hydrogen bonds in the structure of the title compound. The one-dimensional chains are joined by these hydrogen bonds to form a three-dimensional framework.

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