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Crystal structure of *poly*[(μ_2 -9*H*-carbazole-3,6-dicarboxylate- $\kappa^4 O^1, O^2: O^3, O^4$)(μ_2 -1,3-di(pyridin-4-yl)propane- $\kappa^2 N: N'$)cadmium(II)] monohydrate, $C_{27}H_{23}N_3O_5Cd$

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Abstract

$C_{27}H_{23}N_3O_5Cd$, monoclinic, $P2_1/n$ (no. 14), $a = 9.6161(7)$ Å, $b = 16.5427(11)$ Å, $c = 15.8900(11)$ Å, $\beta = 105.653(1)^\circ$, $V = 2434.0(3)$ Å³, $Z = 4$, $R_{gt}(F) = 0.0327$, $wR_{ref}(F^2) = 0.0828$, $T = 152(2)$ K.

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A part of the molecular 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.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	$0.26 \times 0.25 \times 0.22$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.94 mm^{-1}
Diffractometer, scan mode:	Apex2, φ and ω
$\theta_{\max}$, completeness:	28.3° , $>99\%$
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	15410, 5948, 0.027
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 4588
$N(\text{param})_{\text{refined}}$:	331
Programs:	Bruker [1], SHELX [2, 3]

Source of material

A mixture of 9*H*-carbazole-3,6-dicarboxylic acid (H_2L) (0.2 mmol), 4-(3-(pyridin-4-yl)propyl)pyridine (0.2 mmol), $CdCl_2 \cdot 2.5(H_2O)$ (0.2 mmol), and H_2O (20 mL) was stirred for ten minutes. The mixture was transferred in a 25 mL stainless steel reactor with a Teflon liner and heated from 298 to 453 K in 5 h and a constant temperature was maintained at 453 K for 72 h. After cooling to room temperature, pink block crystals were collected in 58.7% yield based on Cd.

Experimental details

The U_{iso} values of the hydrogen atoms of parts of carbon group were set to $1.2U_{\text{eq}}(C)$. Hydrogen atoms of water molecules were located from electron density map.

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
C1	0.7966(3)	0.19533(17)	0.84541(16)	0.0356(6)
C2	0.7232(3)	0.21621(16)	0.91397(15)	0.0322(5)
C3	0.7654(3)	0.17707(16)	0.99529(16)	0.0353(6)
H3A	0.8367	0.1359	1.0042	0.042*
C4	0.7064(3)	0.19660(16)	1.06251(16)	0.0363(6)
H4	0.7342	0.1688	1.1168	0.044*
C5	0.6051(3)	0.25817(15)	1.04818(16)	0.0321(5)
C6	0.5566(3)	0.29717(15)	0.96594(15)	0.0313(5)
C7	0.6174(3)	0.27528(16)	0.89904(15)	0.0335(6)
H7	0.5865	0.3007	0.8435	0.040*
C8	0.4555(3)	0.35887(15)	0.97601(15)	0.0316(5)
C9	0.4500(3)	0.35468(15)	1.06382(16)	0.0332(5)
C10	0.3666(3)	0.40879(17)	1.09639(17)	0.0411(6)
H10	0.3627	0.4057	1.1554	0.049*
C11	0.2899(3)	0.46693(17)	1.04088(17)	0.0412(6)
H11	0.2330	0.5045	1.0623	0.049*
C12	0.2937(3)	0.47196(16)	0.95339(16)	0.0345(6)
C13	0.3767(3)	0.41797(15)	0.92107(16)	0.0336(6)
H13	0.3799	0.4213	0.8619	0.040*
C14	0.2094(3)	0.53496(16)	0.89399(18)	0.0382(6)
C15	1.1725(3)	0.00172(17)	0.74655(18)	0.0400(6)
H15	1.0923	−0.0266	0.7106	0.048*
C16	1.3061(3)	−0.03501(18)	0.76672(18)	0.0453(7)
H16	1.3161	−0.0878	0.7455	0.054*
C17	1.4255(3)	0.00490(19)	0.81776(18)	0.0446(7)
C18	1.4014(3)	0.0803(2)	0.84946(19)	0.0500(7)
H18	1.4793	0.1094	0.8867	0.060*
C19	1.2642(3)	0.11322(19)	0.82678(19)	0.0460(7)
H19	1.2504	0.1651	0.8489	0.055*
C20	1.5780(4)	−0.0280(2)	0.8365(2)	0.0670(10)
H20A	1.5762	−0.0783	0.8025	0.080*
H20B	1.6386	0.0117	0.8160	0.080*
C21	1.6462(3)	−0.0457(2)	0.9305(2)	0.0550(8)
H21A	1.6032	−0.0956	0.9471	0.066*
H21B	1.6251	−0.0008	0.9665	0.066*
C22	1.8097(3)	−0.0565(2)	0.9504(2)	0.0545(8)
H22A	1.8524	−0.0058	0.9354	0.065*
H22B	1.8495	−0.0656	1.0140	0.065*
C23	1.8552(3)	−0.12518(17)	0.90210(19)	0.0413(7)
C24	1.9012(3)	−0.11294(19)	0.8285(2)	0.0519(8)
H24	1.8994	−0.0600	0.8050	0.062*
C25	1.9500(3)	−0.17694(19)	0.7883(2)	0.0469(7)
H25	1.9812	−0.1668	0.7374	0.056*
C26	1.9054(3)	−0.26502(18)	0.8883(2)	0.0462(7)
H26	1.9045	−0.3187	0.9094	0.055*
C27	1.8555(3)	−0.20385(18)	0.93116(19)	0.0466(7)
H27	1.8213	−0.2157	0.9806	0.056*
N1	1.1504(2)	0.07537(14)	0.77522(14)	0.0384(5)
N2	1.9549(2)	−0.25264(14)	0.81869(15)	0.0386(5)
N3	0.5363(2)	0.29235(13)	1.10510(13)	0.0359(5)

Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
H3	0.5461	0.2767	1.1593	0.043*
O1	0.9035(2)	0.14850(13)	0.86485(13)	0.0518(5)
O2	0.75157(19)	0.22488(12)	0.76958(11)	0.0425(5)
O3	0.2180(2)	0.53754(12)	0.81603(12)	0.0494(5)
O4	0.1318(2)	0.58407(13)	0.92068(13)	0.0552(6)
OW1	0.0378(4)	0.6251(2)	1.0814(2)	0.0981(10)
Cd1	0.93072(2)	0.14287(2)	0.72699(2)	0.03374(7)
H1A	0.113(2)	0.6379(17)	1.0609(19)	0.051*
H2A	−0.001(3)	0.5898(16)	1.0401(17)	0.051*

Comment

The research of coordination polymers (CPs) is significant and unparalleled for their diversified, designable and tailorable structures as well as unique chemical and physical properties. Over the past decades, CPs have been paid much attention for their great potential applications in many areas [5–8]. Coordination polymers are constructed by incorporating metal cations, anionic and/or neutral linkers. In order to obtain a targeted coordination polymer, it is essential to select appropriate linkers. Polycarboxylates represent one type of anionic linkers for the construction of coordination polymers.

In the title complex, there is one crystallographically independent cadmium(II) ions, one dicarboxylato ligand (L), one 4-(3-(pyridin-4-yl)propyl)pyridine and one water molecule. The cadmium(II) is six-coordinated by four O atoms from two L ligands, and two N atoms from two 4-(3-(pyridin-4-yl)propyl)pyridine ligands to form a distorted octahedron. The distances between Cd and the coordinated atoms are: d(Cd1–N1) = 2.330(2) Å, d(Cd1–N2) = 2.271(2) Å, d(Cd1–O1) = 2.2777(18) Å, d(Cd1–O2) = 2.4270(17) Å, d(Cd1–O3) = 2.2393(18) Å, and d(Cd1–O4) = 2.4581(19) Å, respectively. The Cd(II) coordination angles are in the normal range from 55.22(6)° to 150.69(7)°. The Cd(II) ions are bridged by L ligands and 4-(3-(pyridin-4-yl)propyl)pyridine ligands into a 1D-network. The similar 1D structures have been reported, for example, [Cu(bipa)(py)₂]-0.5(H₂O) prepared from the solvothermal reaction of 5-bromoisophthalic acid, Cu(NO₃)₂·3 H₂O and pyridine, and [Co(p-cpdba)(2,2'-bpy)]_n prepared from 4-(4-carboxyphenylamino)-3,5-dinitrobenzoate acid, CoCl₂·6 H₂O and 2,2'-bipyridine. Both are 1D chain structures through cocoordinating interactions between metal ions with oxygen atoms and nitrogen atoms [9, 10]. In addition, nitrogen ligands are mostly used as the second ligand to obtain more diverse structures. There are many directly related structures with 4-(3-(pyridin-4-yl)propyl)pyridine as nitrogen ligand, such as [11–14].

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