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Crystal structure of *catena*-poly[*diaqua*-bis(μ_2 -4-((4-(pyridin-2-ylmethoxy)phenyl)diazenyl)benzoato- $\kappa^3 O, O': N$)cadmium(II)], $\text{Cd}(\text{C}_{19}\text{H}_{14}\text{O}_3\text{N}_3)_2(\text{H}_2\text{O})$

Table 1: Data collection and handling.

Crystal:	Orange flake
Size:	0.20 × 0.20 × 0.05 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.70 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max} , completeness:	25.0°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	16962, 3019, 0.059
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2641
$N(\text{param})_{\text{refined}}$:	236
Programs:	Bruker [1], SHELX [2]

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Abstract

$\text{C}_{38}\text{H}_{30}\text{N}_6\text{O}_7\text{Cd}$, monoclinic, $C2/c$ (no. 15), $a = 16.937(3)$ Å, $b = 6.1323(12)$ Å, $c = 33.322(7)$ Å, $\beta = 99.31(3)^\circ$, $V = 3415.4(12)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0314$, $wR_{\text{ref}}(F^2) = 0.0668$, $T = 296(2)$ K.

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A part of the title 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 material

A mixture of 4-(2-(4-((pyridin-2-yl)methoxy)phenyl)diazenyl)benzoic acid (17 mg, 0.04 mmol) and $\text{Cd}(\text{OAc})_2 \cdot 2\text{H}_2\text{O}$ (11 mg, 0.04 mmol) dissolved in DMF (3 mL) and H_2O (1 mL) were placed in a Teflon-lined stainless steel vessel, heated to 413 K for 3 days, and then cooled to room temperature over 24 h. Orange block crystals of 1 were obtained in 42% yield (based on Cd).

Experimental details

The hydrogen atoms were placed in calculated positions riding on attached atoms with isotropic thermal parameters 1.2 times those of their carrier atoms. The U_{iso} values of the

hydrogen atoms of methyl groups and oxygen were set to $1.5U_{\text{eq}}(\text{C}, \text{O})$.

Comment

Metal-organic coordination polymers have attracted considerable attention because of their potential applications as well as their structural diversity and topologies [3–7]. In principle, selection and synthesis of the bridging ligands play a crucial role in the design and construction [8–12]. In comparison to the 1,4-benzenedicarboxylic acid, 1,3,5-benzenetricarboxylic acid, and 1,2,4,5-benzenetetracarboxylic acid ligands, there are only limited known examples of coordination frameworks with 4-(2-(4-((pyridin-2-yl)methoxy)phenyl)diazenyl)benzoic acid or 4-(2-(4-((pyridin-3-yl)methoxy)phenyl)diazenyl)benzoic acid. [13, 14] However, 4-(2-(4-((pyridin-2-yl)methoxy)phenyl)diazenyl)benzoic acid or 4-(2-(4-((pyridin-3-yl)methoxy)phenyl)diazenyl)benzoic acid may provide the potential to construct unpredictable and interesting network structures due to the existence of two rigid benzene ring pieces and two pyridyl arms combined by intervening methoxy, diazene, carbomethoxy groups.

The fundamental unit of the title structure is composed of one half Cd^{II} ions, one 4-(2-(4-((pyridin-2-yl)methoxy)phenyl)diazenyl)benzo anions, and one coordinated water molecule. The Cd1 atom adopts a distorted pentagonal bipyramidal geometry and is seven-coordinated by two nitrogen atoms and four carboxylic oxygen atoms from two 4-(2-(4-((pyridin-2-yl)methoxy)phenyl)diazenyl)benzoate anions as well as one coordinated water molecule. The Cd–N bond lengths is 2.420(2) Å and the Cd–O ones are in the range

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

Atom	x	y	z	U _{iso} [*] /U _{eq}
Cd1	0.5000	0.72504(4)	0.7500	0.02734(10)
C1	0.32526(17)	0.5196(4)	0.72854(9)	0.0380(7)
H1	0.3536	0.4292	0.7482	0.046*
C2	0.24661(19)	0.4701(5)	0.71424(10)	0.0463(8)
H2	0.2228	0.3479	0.7237	0.056*
C3	0.20405(18)	0.6046(5)	0.68575(10)	0.0498(8)
H3	0.1503	0.5774	0.6761	0.060*
C4	0.24193(17)	0.7806(5)	0.67151(9)	0.0443(7)
H4	0.2144	0.8720	0.6518	0.053*
C5	0.32150(16)	0.8190(4)	0.68706(8)	0.0311(6)
C6	0.36535(17)	1.0128(4)	0.67343(8)	0.0344(7)
H6A	0.3726	1.1207	0.6950	0.041*
H6B	0.4180	0.9663	0.6690	0.041*
C7	0.33909(16)	1.0289(4)	0.60055(8)	0.0326(6)
C8	0.37055(18)	0.8234(5)	0.59603(9)	0.0416(7)
H8	0.3823	0.7313	0.6184	0.050*
C9	0.38433(18)	0.7561(5)	0.55830(9)	0.0435(7)
H9	0.4046	0.6175	0.5550	0.052*
C10	0.36798(18)	0.8953(5)	0.52529(9)	0.0392(7)
C11	0.33701(19)	1.1003(5)	0.53033(9)	0.0456(8)
H11	0.3265	1.1944	0.5082	0.055*
C12	0.32160(17)	1.1664(5)	0.56778(9)	0.0403(7)
H12	0.2995	1.3030	0.5709	0.048*
C13	0.41573(18)	0.6024(5)	0.44047(8)	0.0395(7)
C14	0.39917(19)	0.3939(5)	0.42597(9)	0.0460(8)
H14	0.3776	0.2918	0.4418	0.055*
C15	0.41465(17)	0.3372(5)	0.38801(8)	0.0384(7)
H15	0.4029	0.1970	0.3782	0.046*
C16	0.44748(16)	0.4866(4)	0.36438(8)	0.0299(6)
C17	0.46676(16)	0.6926(4)	0.37991(8)	0.0348(7)
H17	0.4905	0.7929	0.3647	0.042*
C18	0.45099(18)	0.7504(4)	0.41781(9)	0.0403(7)
H18	0.4641	0.8891	0.4281	0.048*
C19	0.46250(15)	0.4229(4)	0.32280(8)	0.0288(6)
N1	0.36326(12)	0.6913(3)	0.71569(6)	0.0288(5)
N2	0.38303(16)	0.8440(4)	0.48532(7)	0.0471(7)
N3	0.39695(16)	0.6478(4)	0.48012(7)	0.0467(7)
O1	0.32494(11)	1.1116(3)	0.63721(5)	0.0379(5)
O2	0.48299(12)	0.5666(3)	0.29953(6)	0.0407(5)
O3	0.45450(11)	0.2265(3)	0.31219(6)	0.0375(5)
O1W	0.5000	1.0956(4)	0.7500	0.0506(8)
H1W	0.5021	1.1752	0.7293	0.061*

of 2.272(3) and 2.4816(19) Å. The carboxylate group of 4-(2-(4-((pyridin-2-yl)methoxy)phenyl)diazanyl) benzoate take the chelated bidentate mode to Cd^{II}. On the basis of this connection, the [Cd(H₂O)] subunits are linked by carboxylate groups and N atoms, respectively, resulting in a chain. The Cd–Cd distances across linkers is 16.88 Å.

References

1. BRUKER. SAINT, APEX2 and SADABS. Bruker AXS Inc., Madison, WI, USA (2009).

2. Sheldrick, G. M.: Crystal structure refinement with *SHELXL*. *Acta Crystallogr.* **C71** (2015) 3–8.
3. Ma, L.-F.; Han, M.-L.; Qin, J.-H.; Wang, L.-Y.; Du, M.: Mn^{II} coordination polymers based on bi-, tri-, and tetranuclear and polymeric chain building units: crystal structures and magnetic properties. *Inorg. Chem.* **51** (2012) 9437–9442.
4. Han, M.-L.; Wang, J.-G.; Ma, L.-F.; Guo, H.; Wang, L.-Y.: Construction of Cd(II) coordination polymers based on R-isophthalate (R = –CH₃ or –OCH₃) and flexible N-donor co-ligands: syntheses, structures and photoluminescence. *CrystEngComm* **14** (2012) 2691–2701.
5. Wang, Y.; Wang, L.; Zhou, X.; Li, Y.; Li, J.: Three Cd(II) complexes based on pyridine containing mercaptotriazole and aromatic multi-carboxylates: syntheses, structures and luminescent properties. *J. Mol. Struct.* **1173** (2018) 612–619.
6. Zhang, G. Y.; Zhou, X. L.; Li, T.; Meng, X. R.: Three Cd^{II} complexes based on 2-(1*H*-imidazol-1-methyl)-1*H*-benzimidazole and homologous aliphatic dicarboxylates. *Inorg. Chim. Acta* **421** (2014) 45–51.
7. Sun, D.; Li, Y. H.; Hao, H. J.; Liu, F. J.; Zhao, Y.; Huang, R. B.; Zheng, L. S.: Syntheses, structures and photoluminescent properties of a series of Ag(I) coordination architectures based on 2,4-diamino-6-methyl-1,3,5-triazine and dicarboxylates: from a 0D discrete molecule to a 3D infinite network. *CrystEngComm* **13** (2011) 6431–6441.
8. Liu, L.-L.; Yu, C.-X.; Ma, F.-J.; Li, Y.-R.; Han, J.-J.; Lu, L.; Ma, L.-F.: Structural diversity and photocatalytic properties of Cd(II) coordination polymers constructed by a flexible V-shaped bipyridyl benzene ligand and dicarboxylate derivatives. *Dalton Trans.* **44** (2015) 1636–1645.
9. Chun, H.; Dybtsev, D. N.; Kim, H.; Kim, Kimoon.: Synthesis, X-ray crystal structures, and gas sorption properties of pillared square grid nets based on paddle-wheel motifs: implications for hydrogen storage in porous materials. *Chem. Eur. J.* **11** (2005) 3521–3529.
10. Zou, G. D.; Huo, X. X.; Yu, X. C.; Tang, L.; Zhang, B.; Huang, X. Y.: Three transition metal cluster-based coordination polymers based on 1,4-naphthalene dicarboxylate and pyridine ligands. *Inorg. Chem. Commun.* **74** (2016) 16–21.
11. Shi, L. L.; Zhang, Y. Q.; Han, S. S.; Yang, Z. Z.; Zhu, L. M.; Li, B. L.; Li, H. Y.: Syntheses, structures, properties of a series of coordination polymers with flexible bis(imidazole) and dicarboxylate ligands. *Polyhedron* **133** (2017) 82–91.
12. Park, I.; Medishetty, R. E.; Lee, H. H.; Herng, T. S.; Ding, J.; Lee, S. S.; Vittal, J. J.: Influence of angular dicarboxylate ligand on the structures of single and double pillared-layer coordination polymers of Co(II). *Cryst. Growth Des.* **15** (2015) 4156–4161.
13. Liu, L. L.; Yu, C. X.; Du, J. M.; Liu, S. M.; Cao, J. S.; Ma, L. F.: Construction of five Zn(II)/Cd(II) coordination polymers derived from a new linear carboxylate/pyridyl ligand: design, synthesis, and photocatalytic properties. *Dalton Trans.* **45** (2016) 12352–12361.
14. Yu, Y. Z.; Chang, S. Y.; Han, X.; Chen, G. X.; Xuan, Y. W.; Wu, X. L.; Wang, F.: Hydrothermal synthesis, crystal structure and luminescence property of a 2D manganese(II) coordination polymer. *Chin. J. Struct. Chem.* **38** (2019) 147–154.