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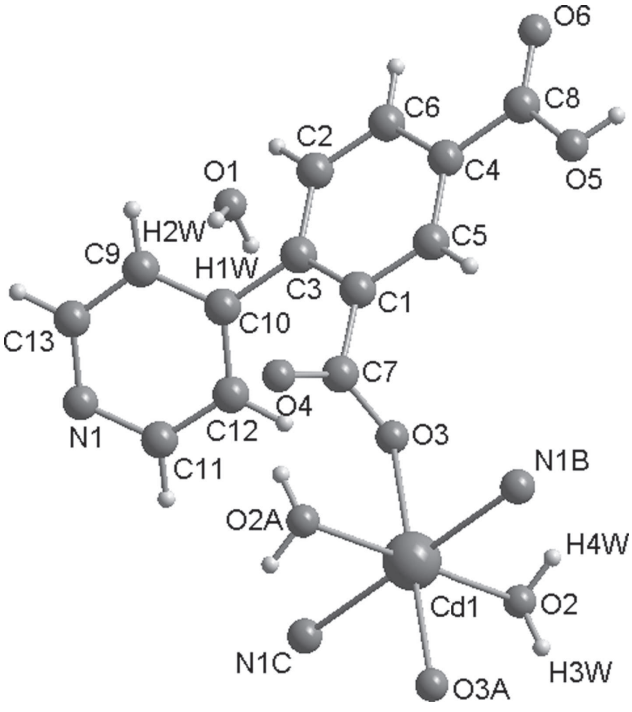
Yan Zhao* and Dai-Jian Guo

Crystal structure of catena-poly[diaqua-bis-(μ$_2$-5-carboxy-2-(pyridin-4-yl)benzoato-κ^2*O*:*N*) cadmium(II)] dihydrate, $C_{26}H_{24}N_2O_{12}Cd$



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Abstract

$C_{26}H_{24}N_2O_{12}Cd$, triclinic, $P\bar{1}$, $a = 6.9812(9)$ Å, $b = 8.6834(11)$ Å, $c = 11.5157(15)$ Å, $\alpha = 86.649(10)^o$, $\beta = 88.686(10)^o$, $\gamma = 85.008(10)^o$, $V = 694.14(15)$ Å^3, $Z = 1$, $R_{gt}(F) = 0.0271$, $wR_{ref}(F^2) = 0.0815$, $T = 293(2)$ K.

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The crystal structure is shown in the figure, Tables 1–3 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

***Corresponding author: Yan Zhao,** College of Physics and Electronic Information, Luoyang Normal University, Luoyang 471022, Henan Province, P. R. China, e-mail: zhanglihxx@126.com
Dai-Jian Guo: Department of Life Science, Luoyang Normal University, Luoyang 471022, Henan Province, P. R. China

Table 1: Data collection and handling.

Crystal:	Colourless, block, size 0.32×0.34×0.35 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	8.53 cm^{-1}
Diffractometer, scan mode:	CCD area detector, φ and ω scans
$2\theta_{max}$:	51°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	4974, 2516
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2512
$N(param)_{refined}$:	188
Programs:	SHELX [7]

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

Atom	Site	*x*	*y*	*z*	U_{iso}
H(1W)	2*i*	0.5684	0.2575	0.2482	0.062
H(2W)	2*i*	0.7627	0.2030	0.2773	0.062
H(3W)	2*i*	−0.3543	−0.0885	0.4870	0.056
H(4W)	2*i*	−0.2746	−0.0658	0.3764	0.056
H(5)	2*i*	0.2775	−0.1051	−0.1253	0.073
H(2)	2*i*	0.2416	0.5852	0.0036	0.037
H(5A)	2*i*	0.2136	0.0658	0.1154	0.035
H(6)	2*i*	0.2857	0.4027	−0.1328	0.037
H(9)	2*i*	0.3779	0.6966	0.1743	0.045
H(11)	2*i*	−0.1021	0.6604	0.4482	0.041
H(12)	2*i*	−0.0502	0.4685	0.3207	0.037
H(13)	2*i*	0.3162	0.8808	0.3082	0.046

Source of material

A mixture of $Cd(NO_3)_2{\cdot}2H_2O$ (0.1 mmol, 0.0272 g), 4-(pyridin-4-yl)-isophthalic acid (0.1 mmol, 0.0243 g) and distilled water (10 mL) was heated in a 25 mL stainless steel reactor with a Teflon liner at 423 K for 36 h, followed by slow cooling to room temperature. Colourless crystals of the compound formed.

Discussion

In recent years, research on coordination complexes has made considerable progress in the fields of supramolecular chemistry and crystal engineering, owing to their intriguing architectures and functional applications, such as gas storage

Table 3: Atomic displacement parameters (Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cd(1)	1*b*	0	0	0.5	0.0379(2)	0.0206(2)	0.0227(2)	−0.0021(1)	0.0033(1)	−0.0050(1)
N(1)	2*i*	0.1006(3)	0.7903(3)	0.3907(2)	0.044(1)	0.023(1)	0.031(1)	−0.0019(9)	0.006(1)	−0.0084(9)
O(1)	2*i*	0.6870(3)	0.2531(3)	0.2291(2)	0.045(1)	0.040(1)	0.039(1)	−0.0034(9)	−0.0008(9)	−0.0065(9)
O(2)	2*i*	−0.3113(3)	−0.0222(2)	0.4382(2)	0.039(1)	0.042(1)	0.030(1)	−0.0041(9)	0.0039(8)	−0.0079(9)
O(3)	2*i*	0.0388(3)	0.1592(2)	0.3368(2)	0.041(1)	0.035(1)	0.028(1)	−0.0080(8)	0.0049(8)	0.0043(8)
O(4)	2*i*	0.3339(3)	0.2291(3)	0.3641(2)	0.042(1)	0.057(1)	0.029(1)	−0.008(1)	−0.0038(9)	0.008(1)
O(5)	2*i*	0.2741(4)	−0.0474(3)	−0.0713(2)	0.082(2)	0.034(1)	0.033(1)	−0.008(1)	0.010(1)	−0.0125(9)
O(6)	2*i*	0.3188(4)	0.1322(3)	−0.2145(2)	0.076(2)	0.046(1)	0.025(1)	−0.014(1)	0.010(1)	−0.0116(9)
C(1)	2*i*	0.2003(3)	0.2791(3)	0.1772(2)	0.029(1)	0.024(1)	0.023(1)	−0.0020(9)	0.0033(9)	−0.003(1)
C(2)	2*i*	0.2377(4)	0.4811(3)	0.0266(2)	0.039(1)	0.025(1)	0.028(1)	−0.001(1)	0.006(1)	0.002(1)
C(3)	2*i*	0.2065(4)	0.4382(3)	0.1447(2)	0.029(1)	0.023(1)	0.025(1)	−0.0005(9)	0.0034(9)	−0.003(1)
C(4)	2*i*	0.2535(4)	0.2145(3)	−0.0233(2)	0.031(1)	0.032(1)	0.024(1)	−0.003(1)	0.003(1)	−0.007(1)
C(5)	2*i*	0.2212(4)	0.1699(3)	0.0935(2)	0.037(1)	0.025(1)	0.027(1)	−0.005(1)	0.004(1)	−0.004(1)
C(6)	2*i*	0.2626(4)	0.3719(3)	−0.0554(2)	0.036(1)	0.035(1)	0.021(1)	−0.002(1)	0.004(1)	−0.000(1)
C(7)	2*i*	0.1908(4)	0.2196(3)	0.3037(2)	0.036(1)	0.019(1)	0.023(1)	0.002(1)	0.005(1)	−0.004(1)
C(8)	2*i*	0.2847(4)	0.0969(3)	−0.1130(2)	0.036(1)	0.036(2)	0.029(2)	−0.005(1)	0.002(1)	−0.010(1)
C(9)	2*i*	0.2799(4)	0.6860(3)	0.2295(3)	0.041(2)	0.031(1)	0.042(2)	−0.007(1)	0.015(1)	−0.010(1)
C(10)	2*i*	0.1722(4)	0.5583(3)	0.2312(2)	0.033(1)	0.023(1)	0.026(1)	0.002(1)	0.002(1)	−0.003(1)
C(11)	2*i*	−0.0042(4)	0.6674(3)	0.3925(2)	0.044(2)	0.027(1)	0.031(1)	−0.002(1)	0.012(1)	−0.005(1)
C(12)	2*i*	0.0262(4)	0.5513(3)	0.3160(2)	0.041(1)	0.021(1)	0.032(1)	−0.004(1)	0.008(1)	−0.004(1)
C(13)	2*i*	0.2410(4)	0.7973(3)	0.3102(3)	0.041(2)	0.027(1)	0.048(2)	−0.008(1)	0.009(1)	−0.012(1)

[1], catalysis [2], magnetism [3] and luminescence [4]. Studies in this field have been focused on the rational design and synthesis of novel frameworks and the relationships between their structures and properties. The observation of coordination complexes constructed from organic ligands and metal ions through a self-assembly route has been explored intensively, and many efforts have been devoted to use of N- and O-donor organic ligands as co-ligands to bridge metal ions to form infinite network structures, such as one-dimensional (1D) chain structures and 2- or 3-D networks [5]. However, it is still a great challenge in crystal engineering to obtain designed and predictable frameworks with potential properties assembled by coordination bonds and/or weak supramolecular interactions such as hydrogen bonds, π–π stacking, and host–guest ionic interactions, etc. [6].

The asymmetric unit of the title structure contains one half of a Co(II) metal center, two water molecules and one organic monoanion as a bridging ligand to construct a new coordination polymer. The cadmium atom is six-coordinated by two water ligands, two oxygen atoms from two 5-carboxy-2-(pyridin-4-yl)benzoato ligands and two nitrogen atoms from two other symmetry related organic ligands. The Cd—O bond lengths are 2.2921(19) Å and 2.329(2) Å. The bond angles of O—Cd—O are in the range of 87.10(7)° to 180°. All moieties are connected by hydrogen bonds d(O(1)—H(2W)···O(3)#7) = 2.812(3) Å, d(O(1)—H(1W)···O(4)) = 2.900(3) Å, d(O(5)—H(5)···O(1)#5) = 2.615(3) Å d(O(2)—H(4W)···O(6)#6) = 2.803(3) Å, d(O(2)—H(3W)···O(4)#1) = 2.827(3) Å. Symmetry codes: #1 $-x$, $-y$, $-z+1$; #5 $-x+1$, $-y$, $-z$; #6 $-x$, $-y$, $-z$; #7 $x+1$, y, z. These hydrogen bonds result in a 3D framework.

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