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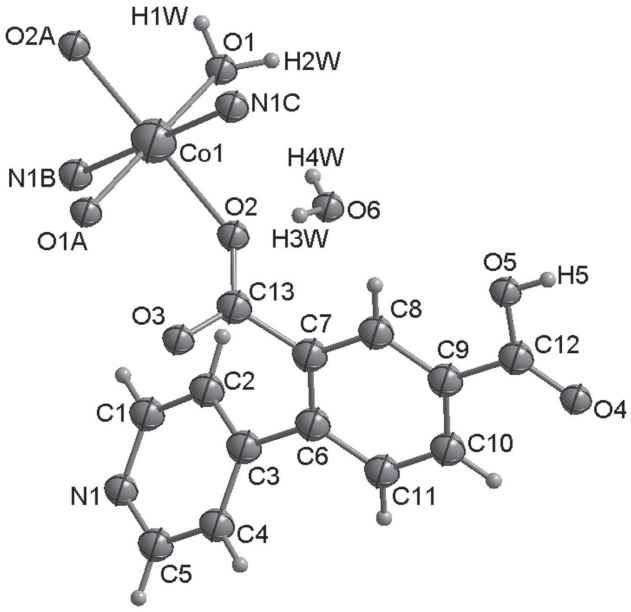
Crystal structure of catena-poly[diaqua-bis(μ_2-5-carboxy-2-(pyridin-4-yl)benzoato-κ_2O:N)-cobalt(II)]dihydrate, $C_{26}H_{24}N_2O_{12}Co$



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Abstract

$C_{26}H_{24}N_2O_{12}Co$, triclinic, $P\bar{1}$, $a = 6.892(3)$ Å, $b = 8.469(4)$ Å, $c = 11.306(5)$ Å, $\alpha = 86.963(6)°$, $\beta = 88.691(5)°$, $\gamma = 85.404(6)°$, $V = 694.14(15)$ Å^3, $Z = 1$, $R_{gt}(F) = 0.0561$, $wR_{ref}(F^2) = 0.1319$, $T = 293(2)$ 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.

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Table 1: Data collection and handling.

Crystal:	Red, block, size 0.25×0.32×0.41 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	7.24 cm^{-1}
Diffractometer, scan mode:	CCD area detector, φ and ω scans
$2\theta_{max}$:	51°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	4061, 2354
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1548
$N(param)_{refined}$:	188
Programs:	SHELXL [9]

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*	0.8277	0.5859	0.0064	0.040
H(2W)	2*i*	0.8254	0.5437	0.1212	0.040
H(5)	2*i*	0.2258	0.6182	0.6265	0.066
H(3W)	2*i*	0.7018	0.2746	0.2296	0.049
H(4W)	2*i*	0.8949	0.2419	0.2244	0.049
H(1A)	2*i*	0.6150	−0.1676	0.0481	0.033
H(2)	2*i*	0.5571	0.0322	0.1753	0.031
H(4)	2*i*	0.1110	−0.1943	0.3116	0.038
H(5A)	2*i*	0.1782	−0.3889	0.1788	0.037
H(8)	2*i*	0.2912	0.4441	0.3811	0.031
H(10)	2*i*	0.2204	0.1002	0.6328	0.033
H(11)	2*i*	0.2567	−0.0877	0.4909	0.032

Experimental details

A mixture of $Co(NO_3)_2$ $6H_2O$ (0.1 mmol, 267 mg), 4-(pyridin-4-yl)-isophthalic acid (0.1 mmol, 24.3 mg) (H2tpa) and distilled water (10 mL) was heated in a 25 mL stainless steel reactor with a Teflon liner at 413 K for 24 h, followed by slow cooling to room temperature to formed crystals.

Results and discussion

The design and construction of metal-organic frameworks (MOFs) with well-regulated network structures has been

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

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Co(1)	1*e*	0.5	0.5	0.0	0.0234(6)	0.0218(6)	0.0146(5)	−0.0009(4)	0.0017(4)	−0.0009(4)
N(1)	2*i*	0.4057(6)	−0.2992(5)	0.1007(3)	0.031(2)	0.023(3)	0.022(2)	0.002(2)	0.003(2)	−0.005(2)
O(1)	2*i*	0.7868(5)	0.5156(4)	0.0552(3)	0.032(2)	0.029(2)	0.020(2)	−0.004(2)	−0.002(2)	−0.001(2)
O(2)	2*i*	0.4569(5)	0.3535(4)	0.1533(3)	0.026(2)	0.029(2)	0.022(2)	−0.006(2)	0.002(1)	0.003(2)
O(3)	2*i*	0.1596(5)	0.2745(4)	0.1301(3)	0.030(2)	0.042(2)	0.024(2)	−0.011(2)	−0.001(2)	0.006(2)
O(4)	2*i*	0.1868(6)	0.3751(5)	0.7171(3)	0.061(3)	0.042(3)	0.019(2)	−0.009(2)	0.008(2)	−0.008(2)
O(5)	2*i*	0.2295(7)	0.5585(5)	0.5715(3)	0.075(3)	0.035(3)	0.024(2)	−0.009(2)	0.008(2)	−0.010(2)
O(6)	2*i*	0.8077(5)	0.2397(4)	0.2623(3)	0.034(2)	0.038(2)	0.026(2)	−0.002(2)	0.000(2)	−0.003(2)
C(1)	2*i*	0.5119(7)	−0.1734(6)	0.1023(4)	0.028(3)	0.027(3)	0.028(3)	−0.005(2)	0.009(2)	−0.002(2)
C(2)	2*i*	0.4785(7)	−0.0522(6)	0.1786(4)	0.032(3)	0.022(3)	0.023(3)	−0.003(2)	0.005(2)	−0.002(2)
C(3)	2*i*	0.3257(7)	−0.0582(6)	0.2606(4)	0.027(3)	0.023(3)	0.015(2)	0.003(2)	0.003(2)	−0.004(2)
C(4)	2*i*	0.2152(8)	−0.1864(6)	0.2585(4)	0.032(3)	0.033(3)	0.029(3)	−0.002(3)	0.012(2)	−0.006(2)
C(5)	2*i*	0.2564(7)	−0.3044(6)	0.1784(4)	0.031(3)	0.027(3)	0.034(3)	−0.003(2)	0.006(2)	−0.006(2)
C(6)	2*i*	0.2931(7)	0.0655(6)	0.3502(4)	0.022(3)	0.023(3)	0.023(3)	0.000(2)	0.004(2)	−0.004(2)
C(7)	2*i*	0.2992(7)	0.2264(6)	0.3171(4)	0.022(3)	0.023(3)	0.013(2)	−0.002(2)	0.001(2)	0.001(2)
C(8)	2*i*	0.2815(7)	0.3375(6)	0.4027(4)	0.029(3)	0.023(3)	0.023(3)	−0.003(2)	0.003(2)	0.002(2)
C(9)	2*i*	0.2491(7)	0.2907(6)	0.5217(4)	0.023(3)	0.029(3)	0.021(3)	−0.002(2)	0.003(2)	−0.006(2)
C(10)	2*i*	0.2408(7)	0.1319(6)	0.5538(4)	0.030(3)	0.037(4)	0.016(2)	−0.001(2)	0.006(2)	−0.003(2)
C(11)	2*i*	0.2625(7)	0.0191(6)	0.4687(4)	0.032(3)	0.025(3)	0.022(3)	0.000(2)	0.002(2)	0.005(2)
C(12)	2*i*	0.2220(7)	0.4110(6)	0.6139(4)	0.028(3)	0.024(3)	0.030(3)	0.001(2)	0.002(2)	−0.007(2)
C(13)	2*i*	0.3065(7)	0.2872(6)	0.1901(4)	0.026(3)	0.019(3)	0.018(2)	0.000(2)	0.004(2)	0.000(2)

provoked significant interest on these functional materials with various application fields, e.g. in electrochemistry, photophysics, catalysis, adsorption and separation [1–4]. The organic ligands, which have their differences in the size, the flexibility, the coordination ability, the number of the carboxylate groups, the positions of the carboxylate groups and so on, play crucial role in the design and construction of desirable frameworks with interesting properties [5–8]. In addition, N-containing auxiliary ligands are known to be ideal connectors between metal atoms for the propagation of coordination networks. With these considerations in mind, we have chosen the Htpa as bridging ligands to construct a new complex.

The asymmetric unit of the title structure contains one half of a Co(II) metal center, two water molecules and one Htpa monoanion as bridging ligands to construct a new coordination polymer. The cobalt atom is six-coordinated [CoN_2O_4] in a distorted octahedral manner by two water ligands, two oxygen atoms from two Htpa ligands and two nitrogen atoms from two other symmetry related Htpa ligands. The Co–O bond lengths range from 2.10–2.19 Å. The bond angles of O—Co—O are in the range of 87.73(12)° to 180°. In addition, coordinated and uncoordinated water molecules are connected with 4-(pyridin-4-yl)-isophthalic ligands by hydrogen bonds: d(O6—H4W$\cdots$O3#5) = 2.847(5) Å, d(O6—H3W$\cdots$O2) = 2.815(5) Å, d(O1—H2W$\cdots$O4#6) = 2.797(5) Å, d(O1—H1W$\cdots$O3#1) = 2.713(5) Å. Symmetry codes: #1 $-x+1$, $-y+1$, $-z$; #5 $x+1$, y, z; #6 $-x+1$, $-y+1$, $-z+1$. These interactions result in the infinite three dimensional architecture of the title structure.

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