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Crystal structure of poly[diaqua-bis(μ_2 -3-(pyrimidin-5-yl)benzoato- $\kappa^2 N:O$)cobalt(II)] dihydrate, $[\text{Co}(\text{C}_{11}\text{H}_{11}\text{O}_2\text{N}_2)_2(\text{H}_2\text{O})_2]$

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Abstract

$[\text{Co}(\text{C}_{11}\text{H}_{11}\text{O}_2\text{N}_2)_2(\text{H}_2\text{O})_2]$, monoclinic, $P2_1/c$ (no. 14),
 $a = 8.7117(5)$ Å, $b = 8.7935(5)$ Å, $c = 15.0791(9)$ Å,

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	$0.13 \times 0.11 \times 0.10$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.82 mm^{-1}
Diffractometer, scan mode:	φ and ω
θ_{max} , completeness:	28.3° , >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	6839, 2676, 0.018
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2340
$N(\text{param})_{\text{refined}}$:	172
Programs:	Bruker [1], SHELX [2, 3], Diamond [4]

$\beta = 103.557(1)^\circ$, $V = 1122.97(11) \text{ \AA}^3$, $Z = 2$, $R_{\text{gt}}(F) = 0.0271$,
 $wR_{\text{ref}}(F^2) = 0.0725$, $T = 296(2) \text{ K}$.

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The asymmetric unit 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.

Source of material

All reagents and solvents employed were commercially available and used as received without further purification. The title compound was synthesized *via* the reaction of $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (0.0125 mmol, 0.00375 g), 3-(pyrimidin-5-yl) benzoic acid (0.025 mmol, 0.005 g) in 1 mL dimethylformamide (DMF) and 0.5 mL water. The mixture was stirred for 0.5 h and then heated at 85°C for 12 h to afford pink block crystals in a yield of 75%.

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

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

Atom	x	y	z	<i>U</i> _{iso} */ <i>U</i> _{eq}
Co1	0.500000	0.000000	1.000000	0.02176 (9)
O1	0.85551 (13)	0.61825 (15)	0.62114 (7)	0.0381 (3)
O2	0.61420 (13)	0.55215 (14)	0.63417 (7)	0.0309 (2)
O3	0.30785 (14)	0.05714 (15)	1.04896 (8)	0.0337 (3)
N1	0.58426 (15)	0.23641 (14)	1.02250 (8)	0.0261 (3)
N2	0.66254 (16)	0.42948 (16)	1.13396 (8)	0.0318 (3)
C1	0.59837 (18)	0.29584 (18)	1.10563 (10)	0.0300 (3)
H1	0.559756	0.238383	1.147422	0.036*
C2	0.71720 (19)	0.51054 (18)	1.07325 (10)	0.0295 (3)
H2	0.761698	0.605149	1.090892	0.035*
H3A	0.273 (3)	0.008 (2)	1.0857 (15)	0.044*
H3B	0.240 (2)	0.075 (2)	1.0049 (15)	0.044*
H4A	0.089 (3)	−0.108 (2)	1.1610 (14)	0.044*
H4B	0.225 (2)	−0.087 (3)	1.2178 (14)	0.044*
C3	0.71114 (17)	0.46087 (17)	0.98465 (10)	0.0238 (3)
C4	0.64096 (17)	0.31990 (17)	0.96275 (9)	0.0253 (3)
H4	0.632849	0.281685	0.904326	0.030*
C5	0.78163 (17)	0.55104 (17)	0.92096 (9)	0.0231 (3)
C6	0.90470 (17)	0.65317 (17)	0.95550 (10)	0.0259 (3)
H6	0.940460	0.664648	1.018269	0.031*
C7	0.97358 (17)	0.73690 (18)	0.89783 (10)	0.0280 (3)
H7	1.052437	0.806847	0.921865	0.034*
C8	0.92587 (17)	0.71724 (18)	0.80447 (10)	0.0278 (3)
H8	0.974695	0.771593	0.765835	0.033*
C9	0.80438 (17)	0.61574 (17)	0.76837 (9)	0.0246 (3)
C10	0.73136 (17)	0.53534 (17)	0.82673 (10)	0.0247 (3)
H10	0.647911	0.470317	0.802415	0.030*
C11	0.75461 (17)	0.59345 (16)	0.66665 (9)	0.0251 (3)
O4	0.18901 (17)	−0.10870 (17)	1.16861 (9)	0.0438 (3)

Comment

2-D metal-organic frameworks (MOFs) and coordination polymers (CP) have drawn tremendous attentions because of their great enormous potential applications in energy storage [5, 6], catalysis [7], as well as sensor [8].

In this work, we synthesize a 2D CP constructed by central Co ions and the 3-(pyrimidin-5-yl)benzoate (L) ligand under solvothermal conditions. L is an efficient ligand which contains benzoate and pyrimidine functional groups. Surprisingly, compounds based on HL are reported uncommonly.

The structure of this compound is centrosymmetric with Co²⁺ on the inversion center. The Co center is coordinated by two N atoms from two L and four O atoms from two L and two coordinated water molecules (see the

Figure). The distances of Co–O bonds are 2.00443(11) Å, 2.0856(10) Å, and the distances of the Co–N bonds are 2.2043(13) Å. Interestingly, the dihedral angle between the benzene ring and the pyrimidine ring is 24.7°. What's more, there are $\pi \cdots \pi$ stacking interactions between the aromatic rings, to construct a three-dimensional architecture. Finally, it should be mentioned that an isomorphous structure is already known [9].

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