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Crystal structure of poly[μ_3 -5-(4-(2,6-di(pyridine-2-yl)pyridine-4-yl)phenoxy)isophthalato- $\kappa^6 O:O',O'':N,N',N''$ cobalt(II)]

$C_{29}H_{17}CoN_3O_5$

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Abstract

$C_{29}H_{17}CoN_3O_5$, monoclinic, $P2_1$ (no. 4), $a = 7.7751(6)$ Å, $b = 12.8081(14)$ Å, $c = 12.4032(15)$ Å, $\beta = 103.79(1)^\circ$, $V = 1199.6(2)$ Å³, $Z = 2$, $R_{gt}(F) = 0.0627$, $wR_{ref}(F^2) = 0.0940$, $T = 293(2)$ K.

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The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of materials

The title complex was synthesized solvothermally in a Teflon-lined stainless steel container by heating a mixture of H_2L (0.0146 g, 0.03 mmol), $Co(NO_3)_2 \cdot 6H_2O$ (0.0087 g, 0.03 mmol) in 6 mL of distilled water at 120 °C for 3 days under auto-genous pressure. Subsequent cooling to room temperature yielded red block crystals.

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Table 1: Data collection and handling.

Crystal:	Red block
Size:	$0.20 \times 0.18 \times 0.16$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.76 mm^{-1}
Diffractometer, scan mode:	New Gemini, φ and ω -scans
$\theta_{\max}$, completeness:	25° , >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	7242, 4138, 0.068
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2826
$N(\text{param})_{\text{refined}}$:	344
Programs:	CrysAlis ^{PRO} [1], SHELX [2]

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

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	1.20879(12)	0.98430(10)	0.65326(10)	0.0380(3)
N1	−0.8259(10)	0.8486(6)	−0.2507(8)	0.044(3)
N2	−0.6176(8)	1.0733(6)	−0.4231(6)	0.0374(19)
N3	−0.5384(8)	0.9520(6)	−0.2519(7)	0.042(2)
O1	0.8279(8)	0.6032(5)	0.2473(6)	0.0400(19)
O2	0.6114(10)	0.6545(6)	0.1080(6)	0.075(3)
O3	1.1215(7)	0.8898(5)	0.5019(6)	0.055(2)
O4	0.9470(6)	0.9979(6)	0.5587(5)	0.055(2)
O5	0.3899(6)	0.9888(6)	0.2570(5)	0.0497(16)
C1	0.6973(11)	0.7686(6)	0.2571(7)	0.033(2)
C2	0.8331(11)	0.8018(7)	0.3473(7)	0.035(2)
H2	0.932451	0.759909	0.371738	0.042*
C3	0.8213(10)	0.8941(7)	0.3993(8)	0.034(2)
C4	0.6713(10)	0.9563(6)	0.3678(7)	0.040(3)
H4	0.662683	1.018823	0.404246	0.048*
C5	0.5329(10)	0.9227(7)	0.2798(7)	0.034(2)
C6	0.5469(10)	0.8305(6)	0.2256(7)	0.033(2)
H6	0.454695	0.809410	0.167200	0.039*
C7	0.2483(9)	0.9670(9)	0.1659(7)	0.041(3)
C8	0.2507(10)	0.9988(9)	0.0654(8)	0.049(3)
H8	0.353826	1.028026	0.053164	0.058*
C9	0.1019(9)	0.9897(9)	−0.0235(7)	0.044(2)
H9	0.105642	1.015123	−0.093114	0.053*
C10	−0.0509(10)	0.9427(7)	−0.0078(8)	0.039(3)
C11	−0.0465(12)	0.9056(9)	0.0969(9)	0.061(3)
H11	−0.146257	0.872169	0.109332	0.073*
C12	0.1022(11)	0.9161(8)	0.1854(9)	0.056(3)
H12	0.102595	0.889641	0.255240	0.067*
C13	−0.2187(10)	0.9408(7)	−0.0955(8)	0.039(3)
C14	−0.2424(10)	1.0078(7)	−0.1881(8)	0.042(3)
H14	−0.149965	1.050149	−0.197523	0.050*

Table 2 (Continued)

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C15	−0.4039(10)	1.0103(7)	−0.2648(7)	0.036(3)
C16	−0.5176(11)	0.8836(7)	−0.1704(9)	0.042(3)
C17	−0.3591(11)	0.8751(7)	−0.0904(8)	0.047(3)
H17	−0.346979	0.825894	−0.033982	0.057*
C18	−0.6797(13)	0.8190(8)	−0.1694(10)	0.045(3)
C19	−0.6877(14)	0.7389(8)	−0.0983(10)	0.067(4)
H19	−0.587721	0.720126	−0.044131	0.081*
C20	−0.8440(16)	0.6860(10)	−0.1071(12)	0.101(5)
H20	−0.851200	0.631394	−0.058972	0.121*
C21	−0.9914(15)	0.7153(9)	−0.1892(12)	0.087(5)
H21	−1.099164	0.681168	−0.196482	0.105*
C22	−0.9748(12)	0.7943(8)	−0.2581(10)	0.062(3)
H22	−1.073143	0.811896	−0.314152	0.075*
C23	−0.4495(10)	1.0813(7)	−0.3626(8)	0.040(2)
C24	−0.3335(11)	1.1519(7)	−0.3897(8)	0.048(3)
H24	−0.218200	1.157090	−0.346661	0.058*
C25	−0.3901(14)	1.2149(8)	−0.4812(10)	0.055(3)
H25	−0.313256	1.262600	−0.501392	0.066*
C26	−0.5614(13)	1.2061(8)	−0.5421(11)	0.060(4)
H26	−0.602338	1.248415	−0.603831	0.073*
C27	−0.6719(12)	1.1346(8)	−0.5116(9)	0.052(3)
H27	−0.787742	1.128593	−0.553688	0.062*
C28	0.7119(13)	0.6664(8)	0.1988(9)	0.040(3)
C29	0.9728(12)	0.9305(7)	0.4913(8)	0.037(2)

Experimental details

Absorption corrections were applied by using multi-scan program. The structure was refined based on F^2 with the SHELXL [2] software package. Hydrogen atoms attached to C of the title complex located in difference electron density maps, and treated as riding atoms. The U_{iso} values of the hydrogen atoms were set to $1.2U_{\text{eq}}(\text{C})$.

Comment

The construction of inorganic-organic coordination polymers has attracted great attention due to their intriguing architectures [3–6]. Multicarboxylate ligands are excellent candidates, and various coordination polymers based on them have been reported [7]. A rich variety of coordination modes with multicarboxylic groups can be formed and can help to form hydrogen bonding, which extend to high-dimensions. X-ray crystallography analyses reveal that the title complex shows three-dimensional framework linked through hydrogen bonding interactions.

One Co(II) atom and one fully deprotonated L^{2-} ligand can be observed in the asymmetric unit. The Co(II) atom exhibits six-coordinated distorted octahedral geometry, with three nitrogen atoms from one L^{2-} ligand and three oxygen atoms from two different L^{2-} ligands. The Co1–N

bond lengths are from 2.064 to 2.156 Å, and the Co1–O bond lengths fall in the range 2.023(3)–2.176(2) Å, similarly to previous reports [8]. The torsion angle C4–C5–O5–C7 is -176.57° . The two carboxylate groups of the L^{2-} ligand show chelating and monodentate coordination mode, respectively. Adjacent Co1 atoms bridged by the chelating carboxylate group and pyridyl nitrogen atoms of L^{2-} ligand to give rise to an infinite one-dimensional chain. The monodentate carboxylate group connected such chains into two-dimensional layer. The neighboring layers are further linked by hydrogen bonds to form three-dimensional supramolecular network.

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