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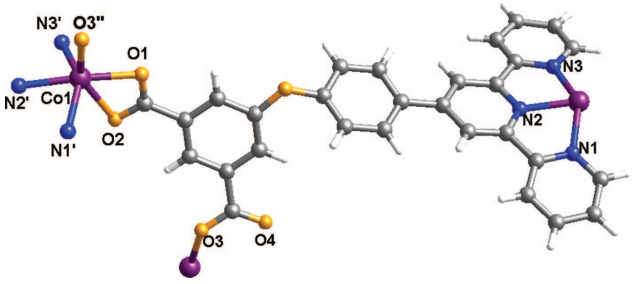
Crystal structure of poly[μ_3-5-(4-(2,6-di(pyridine-2-yl)pyridine-4-yl)phenoxy)isophthalato-κ^5 *O*:*O*′,*O*″:*N*,*N*′,*N*″cobalt(II)], $C_{29}H_{17}CoN_3O_5$



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Abstract

$C_{29}H_{17}CoN_3O_5$, monoclinic, $P2_1/c$ (no. 14), $a = 11.1893(6)$ Å, $b = 13.9922(10)$ Å, $c = 14.1772(7)$ Å, $\beta = 94.544(5)°$, $V = 2212.6(2)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0460$, $wR_{ref}(F^2) = 0.0975$, $T = 293(2)$ K.

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A part of the polymeric title crystal structure is shown in the figure (Symmetry code: ′ = $x-1$, y, $z-1$; ″ = $-x+1$, $y-0.5$, $-z-0.5$). 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 5-(4-(2,6-di(pyridine-2-yl)pyridine-4-yl)phenoxy)isophthalic acid (H_2L, 0.0146 g, 0.03 mmol), $Co(NO_3)_2{\cdot}6H_2O$ (0.0087 g, 0.03 mmol), and 1 mL ethanol and 1 mL DMF in 6 mL of distilled water at 130 °C for 3 days under autogenous pressure.

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Table 1: Data collection and handling.

Crystal:	Red block
Size:	0.20 × 0.18 × 0.16 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.83 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω-scans
θ_{max}, completeness:	25°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	12054, 3902, 0.033
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 3200
$N(param)_{refined}$:	350
Programs:	CrysAlis^{PRO} [1], SHELX [2]

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

Atom	x	y	z	U_{iso}*/U_{eq}
CO1	0.28562(4)	0.33070(3)	−0.32836(3)	0.02661(14)
N1	1.4035(2)	0.3541(2)	0.56109(17)	0.0305(6)
N2	1.1737(2)	0.3647(2)	0.55253(16)	0.0269(6)
N3	1.1168(2)	0.3674(2)	0.72383(16)	0.0293(6)
O1	0.3963(2)	0.31607(18)	−0.20589(16)	0.0470(7)
O2	0.3778(2)	0.46164(18)	−0.25817(15)	0.0402(6)
O3	0.71742(19)	0.68681(16)	−0.15884(14)	0.0347(6)
O4	0.8374(2)	0.6518(2)	−0.03094(16)	0.0542(8)
O5	0.6996(3)	0.3196(2)	0.06312(19)	0.0757(11)
C1	0.5298(3)	0.4316(2)	−0.13351(19)	0.0270(7)
C2	0.5858(3)	0.5192(2)	−0.13988(19)	0.0269(7)
H2	0.557032	0.563022	−0.185496	0.032*
C3	0.6849(3)	0.5423(2)	−0.07858(19)	0.0257(7)
C4	0.7247(3)	0.4772(2)	−0.0087(2)	0.0325(8)
H4	0.789632	0.492370	0.033704	0.039*
C5	0.6686(3)	0.3910(2)	−0.0025(2)	0.0371(9)
C6	0.5712(3)	0.3670(3)	−0.0650(2)	0.0359(8)
H6	0.534184	0.307777	−0.060625	0.043*
C7	0.7801(3)	0.3366(3)	0.1414(2)	0.0477(10)
C8[a]	0.7344(4)	0.3213(4)	0.2301(3)	0.0441(13)
H8[a]	0.653776	0.307490	0.234506	0.053*
C9[a]	0.8124(3)	0.3275(4)	0.3101(3)	0.0406(13)
H9[a]	0.784578	0.316007	0.369138	0.049*
C8′[b]	0.7425(19)	0.377(2)	0.2198(11)	0.0441(13)
H8′[b]	0.662890	0.394739	0.222924	0.053*
C9′[b]	0.8243(13)	0.390(2)	0.2943(16)	0.0406(13)
H9′[b]	0.802375	0.428656	0.343252	0.049*
C10	0.9348(3)	0.3512(3)	0.3032(2)	0.0372(9)
C11	0.9755(3)	0.3584(3)	0.2147(2)	0.0416(9)
H11	1.056733	0.368844	0.209087	0.050*

Table 2 (continued)

Atom	x	y	z	U_{iso}*/U_{eq}
C12	0.8988(3)	0.3505(3)	0.1337(2)	0.0529(11)
H12	0.928414	0.354727	0.074422	0.063*
C13	1.0184(3)	0.3581(3)	0.3901(2)	0.0324(8)
C14	0.9765(3)	0.3671(3)	0.4793(2)	0.0338(8)
H14	0.894501	0.371507	0.485243	0.041*
C15	1.0555(3)	0.3697(2)	0.5592(2)	0.0283(7)
C16	1.2175(3)	0.3601(2)	0.4676(2)	0.0269(7)
C17	1.1427(3)	0.3555(3)	0.3853(2)	0.0334(8)
H17	1.174975	0.350742	0.326980	0.040*
C18	1.0229(3)	0.3783(2)	0.6583(2)	0.0286(7)
C19	0.9095(3)	0.3980(3)	0.6835(2)	0.0386(9)
H19	0.846590	0.405523	0.637137	0.046*
C20	0.8892(3)	0.4067(3)	0.7775(2)	0.0455(10)
H20	0.812703	0.419333	0.795556	0.055*
C21	0.9846(3)	0.3963(3)	0.8443(2)	0.0434(9)
H21	0.973623	0.403046	0.908344	0.052*
C22	1.0954(3)	0.3760(3)	0.8157(2)	0.0342(8)
H22	1.158784	0.367822	0.861452	0.041*
C23	1.3499(3)	0.3631(2)	0.4727(2)	0.0283(7)
C24	1.4138(3)	0.3817(3)	0.3956(2)	0.0363(8)
H24	1.375110	0.384468	0.335167	0.044*
C25	1.5358(3)	0.3961(3)	0.4091(2)	0.0427(9)
H25	1.580307	0.411659	0.358590	0.051*
C26	1.5903(3)	0.3868(3)	0.4994(3)	0.0422(9)
H26	1.672620	0.395576	0.510566	0.051*
C27	1.5224(3)	0.3645(3)	0.5725(2)	0.0371(9)
H27	1.560588	0.356204	0.632622	0.045*
C28	0.4275(3)	0.4021(3)	−0.2026(2)	0.0314(8)
C29	0.7521(3)	0.6343(2)	−0.0882(2)	0.0289(7)

Occupancies: [a] = 0.853(8), [b] = 0.147(8).

Subsequent cooling to room temperature yielded red block crystals.

Experimental details

Absorption corrections were applied by using multi-scan program. The structure was refined based on F^2 with the SHELXL [3] 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 of water molecules were set to $1.5U_{eq}$(O) and the U_{iso} values of all other hydrogen atoms were set to $1.2U_{eq}$(C).

Comment

Design and synthesis of the metal-organic frameworks have rapidly developed owing not only to their intriguing architectures but also to their potential applications, such as gas storage, magnetism, nonlinear optical activity and catalysis [4–6]. Multicarboxylate ligands are often selected as multifunctional organic linkers to construct interesting structures, and various coordination polymers have been reported [7, 8]. To date, there is only one example based on pyridine carboxylate ligand [3]. H_2L contains both carboxylate and pyridine donor moieties, which can enrich coordination modes. To our knowledge, coordination polymers based on this ligand have been not reported to date. X-ray crystallography analyses reveal that the title complex shows three-dimensional framework linked through hydrogen bonding interactions.

The asymmetric unit contains one Co(II) atom and one fully deprotonated L^{2-} ligand. The geometry around the Co1 atom can be described as a distorted octahedral geometry, and is coordinated by three nitrogen atoms from one L^{2-} ligand and three oxygen atoms form two different L^{2-} ligands. O1, O2, O3 and N2 atoms comprise the equatorial plane, while N1 and N3 occupy the axial positions. The Co1—N bond lengths are from 2.076(2) to 2.152(2) Å, and the Co1—O bond lengths fall in the range 2.021(2)−2.292(2) Å, similarly to previous reports [9, 10]. The two carboxylate groups of the L^{2-} ligand show chelating and monodentate coordination mode, respectively. The chelating carboxylate group and pyridyl nitrogen atoms of L^{2-} ligand bridged adjacent Co1 atoms to give rise to an infinite one-dimensional chain. Adjacent chains are linked through another monodentate carboxylate group to generate two-dimensional layer. The neighboring layers are further linked by hydrogen bonds (C—H—O, H25—O3 2.344(2) Å) to form three-dimensional network.

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