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Crystal structure of *catena*-poly[bis(4-(4-carboxyphenoxy)benzoato- $\kappa^1 O$)- μ_2 -(1,4-bis(1-imidazolyl)benzene- $\kappa^2 N:N'$)cobalt(II)], $C_{40}H_{28}N_4O_{10}Co$

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Abstract

$C_{40}H_{28}N_4O_{10}Co$, monoclinic, $C2/c$ (no. 15), $a = 29.686(3)$ Å, $b = 6.2315(4)$ Å, $c = 21.0994(15)$ Å, $\beta = 114.727(8)^\circ$, $V = 3545.3(5)$ Å³, $Z = 4$, $R_{gt}(F) = 0.0386$, $wR_{ref}(F^2) = 0.0897$, $T = 293(2)$ K.

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Table 1: Data collection and handling.

Crystal:	Purple stick
Size:	$0.20 \times 0.10 \times 0.10$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.55 mm^{-1}
Diffractometer, scan mode:	Xcalibur, ω
$\theta_{\max}$, completeness:	26.0° , >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	7898, 3489, 0.021
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2\sigma(I_{\text{obs}})$, 2994
$N(\text{param})_{\text{refined}}$:	253
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 3]

Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

The mixture of 1,4-bis(1-imidazolyl)benzene (bib; 21 mg; 0.1 mmol), 4,4'-oxydibenzoic acid (26 mg; 0.1 mmol), and $CoCl_2 \cdot 6H_2O$ (24 mg; 0.1 mmol) was dissolved in 10 mL

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$).

Atom	x	y	z	U_{iso}^*/U_{eq}
Co1	1.000000	0.31747 (5)	0.750000	0.02879 (12)
O1	0.94572 (5)	0.1108 (2)	0.73056 (8)	0.0411 (4)
C1	0.90568 (7)	0.2050 (3)	0.72175 (10)	0.0331 (5)
O2	0.90511 (5)	0.3911 (2)	0.74202 (8)	0.0471 (4)
C2	0.85839 (7)	0.0875 (3)	0.68053 (11)	0.0340 (5)
C3	0.85939 (8)	-0.1174 (3)	0.65615 (11)	0.0418 (5)
H1	0.889623	-0.185350	0.667089	0.050*
C4	0.81568 (9)	-0.2220 (4)	0.61558 (12)	0.0501 (6)
H2	0.816288	-0.360238	0.599368	0.060*
C5	0.77149 (9)	-0.1191 (4)	0.59959 (12)	0.0497 (6)
C6	0.76957 (9)	0.0833 (4)	0.62290 (14)	0.0565 (7)
H3	0.739226	0.150801	0.611454	0.068*
C7	0.81320 (8)	0.1863 (4)	0.66363 (13)	0.0481 (6)
H4	0.812207	0.324050	0.679935	0.058*
O3	0.72725 (6)	-0.2174 (3)	0.55523 (8)	0.0663 (6)
C8	0.70533 (8)	-0.3596 (4)	0.58337 (12)	0.0431 (5)
C9	0.66462 (8)	-0.4674 (4)	0.53539 (12)	0.0502 (6)
H5	0.653892	-0.441923	0.487865	0.060*
C10	0.64037 (8)	-0.6119 (4)	0.55876 (12)	0.0481 (6)
H6	0.612702	-0.683077	0.526651	0.058*
C11	0.65604 (7)	-0.6544 (3)	0.62891 (11)	0.0364 (5)
C12	0.69618 (8)	-0.5421 (4)	0.67582 (11)	0.0450 (6)
H7	0.706570	-0.565477	0.723396	0.054*
C13	0.72109 (9)	-0.3961 (4)	0.65333 (12)	0.0495 (6)
H8	0.748401	-0.322786	0.685413	0.059*
C14	0.62991 (8)	-0.8193 (3)	0.65085 (12)	0.0412 (5)
O4	0.59329 (7)	-0.9093 (3)	0.61097 (9)	0.0752 (6)
O5	0.64977 (7)	-0.8593 (3)	0.71782 (9)	0.0588 (5)
H14	0.6295 (12)	-0.955 (5)	0.7291 (17)	0.100 (11)*
N1	1.02428 (6)	0.4870 (3)	0.83929 (8)	0.0344 (4)
C15	1.00141 (8)	0.6385 (3)	0.85747 (11)	0.0393 (5)
H9	0.971148	0.697736	0.827790	0.047*
N2	1.02700 (6)	0.6974 (3)	0.92413 (9)	0.0381 (4)
C16	1.06920 (9)	0.5743 (4)	0.95001 (12)	0.0480 (6)
H10	1.094304	0.578616	0.994979	0.058*
C17	1.06715 (8)	0.4469 (4)	0.89792 (11)	0.0446 (5)
H11	1.091081	0.346323	0.900831	0.053*
C18	1.01303 (8)	0.8523 (3)	0.96262 (11)	0.0393 (5)
C19	1.02476 (9)	0.8157 (3)	1.03218 (12)	0.0464 (6)
H12	1.041509	0.691304	1.053651	0.056*
C20	0.98843 (8)	1.0357 (3)	0.93023 (11)	0.0455 (6)
H13	0.980742	1.059352	0.883309	0.055*

DMF-H₂O solution (V/V, 1:1), giving purple crystals after standing at 50 °C for two weeks (10 mg, 12.8%).

Experimental details

H atoms bound to C atoms were placed in calculated positions and refined as riding on their parent atoms.

Comment

Coordination polymers (CPs) have attracted great attention due to their fascinating topological structures and potential applications [4–6]. Typically, the self-assembly of rational designed organic carboxylates, N-heterocyclic molecules and metal ions is a successful strategy to achieve targeting coordination polymers. 4,4'-oxybis(benzoate) (oba), known as a semi-rigid dicarboxylate ligand, has been extensively utilized to construct coordination polymers because of its strong coordination ability and tunable structure [7–10]. To broaden the coordination chemistry of 4,4'-oxybis(benzoate), in this work, 1,4-bis(1-imidazolyl)benzene (bib) was introduced into the assembling system.

The asymmetric unit of the title complex consists of a half of a Co^{2+} ion, one Hoba[−] ligand, and a half of a bib molecule. Each Co^{2+} ion is four coordinated in a tetrahedron geometry with two oxygen atoms from two Hoba[−] ligands (Co1–O1 = 1.9672(14) Å), and two nitrogen atoms from two bib ligands (Co1–N1 = 2.0123(16) Å). Each Hoba[−] ligand uses one carboxylate group to coordinate to a Co^{2+} ion in a monodentate coordination mode. Each bib ligand coordinates to two Co^{2+} ions using two nitrogen atoms. Thus, a zigzag chain is formed. The neighboring chains are hydrogen bonded with each other through protonated carboxylate groups and uncoordinated oxygen atoms (O5–H14...O2 = 2.636(2) Å) to form a 3D network structure.

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