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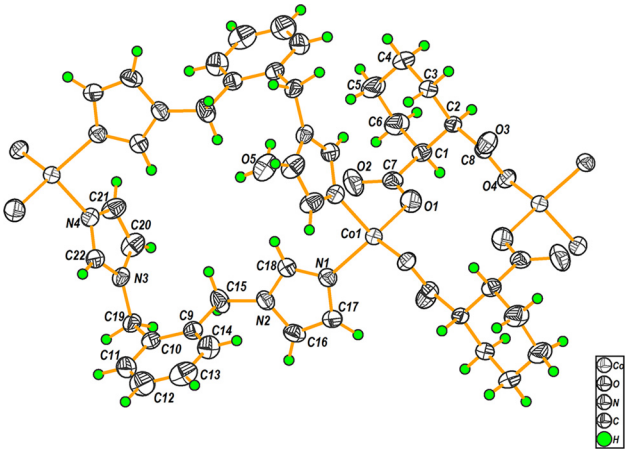
Crystal structure of catena-poly[(μ_2-(2-(1*H*-imidazol-1-ylmethyl)benzyl)-1*H*-imidazole κ^2N:N′)-(μ_2-cyclohexane-1,2-dicarboxylato κ^2O,O′) cobalt(II) monohydrate]



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Abstract

$CoC_{22}H_{26}N_4O_5$, monoclinic, $P2_1/n$, a = 9.531(3) Å, b = 11.771(4) Å, c = 19.673(6) Å, β = 92.495(6)°, V = 2205.0(12) Å^3, Z = 4, $R_{gt}(F)$ = 0.0559 $wR_{ref}(F^2)$ = 0.1253, T = 296(2)K.

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The molecular structure is shown in the figure. Table 1 contains the crystallographic data and the list of the atoms including atomic coordinates and displacement parameters can be found in the cif-file attached to this article.

1 Source of materials

A mixture of $CoCl_2{\cdot}6H_2O$ (0.024 g, 0.1 mmol), 1, 2-bis(imidazole-1-ylmethyl)benzene (1, 2-bib) (0.046 g 0.2 mmol), cyclohexane-1,2-dicarboxylic acid (1,2–DCA) (0.018 g, 0.1 mmol) and H_2O (10 mL) was stirred for about 30 min. The resulting solution was transferred to a Teflon-lined stainless steel autoclave and heated at 393 K for 3 days. After spontaneous cooling to room temperature, red crystals were obtained in approximately 76 % yield based on the cobalt input. The crystals were collected by vacuum filtration and dried in air.

Table 1: Data collection and handling.

Crystal:	Red block
Size:	0.22 × 0.20 × 0.20 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.82 mm^{-1}
Diffractometer, scan mode:	Bruker APEX2, φ and ω scans
θ_{max}, completeness:	28.5°, 100 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	13573, 5422, 0.059
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3,273
$N(param)_{refined}$:	292
Programs:	Bruker,[1] SHELX,[2,3] Olex2[4]

2 Experimental details

The crystal structure was solved using the SHELXT structure solution program within OLEX2 and subsequently refined with the SHELXL refinement package.[2–4]

The C-bound H atoms were geometrically placed (C–H = 0.95 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$.

3 Comment

Coordination polymers (CPs) have recently emerged as a promising class of functional materials in inorganic chemistry and materials science, driven by their structural versatility and tunable properties.[5] These crystalline materials may exhibit exceptional potential in gas storage/separation, heterogeneous catalysis, optoelectronic devices, and biomedical applications, with their multifunctional characteristics continuously inspiring technological advancements.[5–7] The strategic selection of organic ligands-particularly nitrogen-donor heterocycles (e.g., terpyridine derivatives) and carboxylate species-has proven crucial for

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engineering CP architectures.[8,9] Heterocyclic ligands provide multiple coordination sites and enhance framework stability through aromatic stacking interactions, while carboxylate groups contribute strong metal-ligand bonding and structural rigidity. Our group has previously developed a series of imidazole-based CPs using (2-(1H-imidazol-1-ylmethyl)benzyl)-1*H*-imidazole ligands in combination with aromatic carboxylic acids, which exhibited remarkable third-order nonlinear optical responses suitable for photonic applications.[10–14] Systematic variation of ligand substituents and metal centers enables precise control over CP topology and functionality, establishing a robust platform for materials customization. In this work, we report the rational design and synthesis of a coordination polymer, complemented by comprehensive structural characterization via single-crystal X-ray diffraction analysis.

The title compound crystallizes in the monoclinic space group $P2_1/n$, forming a one-dimensional coordination polymer with chain-like topology. The asymmetric unit contains one Co(II) centre, one 1,2-bis(imidazol-1-ylmethyl)benzene (1,2-bib) ligand, one cyclohexane-1,2-dicarboxylic acid (1,2–DCA) ligand, and one lattice water molecule. Structural analysis reveals a distorted tetrahedral coordination geometry about the Co(II) centre, coordinated by two imidazole nitrogen donors from two independent 1,2-bib ligands and two carboxylate oxygen atoms from distinct 1,2–DCA ligands. The Co–N bond lengths are approximately 2.031(3) and 2.055(3) Å, and the Co–O bond lengths are approximately 1.956(3) and 1.983(2) Å. The observed bond lengths correlate well with literature values for similar Co(II) complexes.[11] Notably, an elongated Co(II) and contact of 2.49 Å, suggests weak axial interaction, potentially contributing to the geometric distortion.

The 1,2-bib ligand adopts a *cis*-conformation to bridge symmetry-related Co(II) centres, while each carboxylate group of the 1,2–DCA ligand exhibits monodentate coordination. This bonding pattern generates two distinct metallomacrocycles: a 22-membered ring *via* 1,2-bib bridging (Co⋯Co = 10.19 Å) and a 14-membered ring through 1,2–DCA linkage (Co⋯Co = 5.24 Å). These alternating macrocycles propagate along the crystallographic b-axis, creating the observed 1D polymeric chain. The supramolecular architecture is further stabilized by O–H⋯O hydrogen bonds between lattice water molecules (O1W) and uncoordinated carboxylate oxygens (O2), with d(O⋯O) = 2.82 Å.

Conflict of interest: The authors declare no conflicts of interest regarding this article.

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Author contribution: All the authors have accept-edresponsibility for the entire content of this submitted manuscript and approved submission.

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