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Crystal structure of *catena*-poly(μ2-6-chloropyridine-2-carboxylato-κ^3*N,O:O′*)(6-chloropyridine-2-carboxylato-κ^2*O,N*)copper(II), $C_{12}H_6Cl_2N_2O_4Cu$

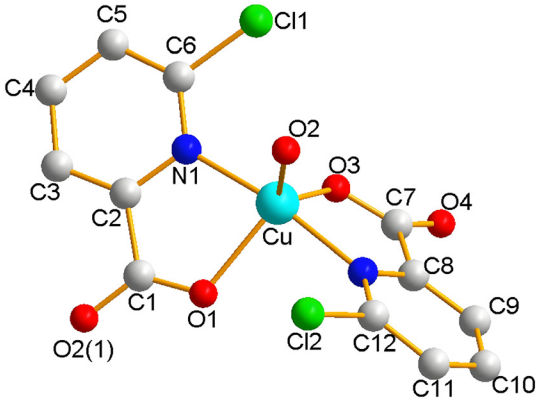

Table 1: Data collection and handling.

Crystal:	Block, green
Size:	0.2 × 0.25 × 0.2 mm
Wavelength:	Mo *K*α radiation, l = 0.71073 Å
μ:	2.04 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω scans
θ_{max}, completeness:	27.1°, >99.9 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	8931, 2971, 0.0181
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2,780
$N(param)_{refined}$:	190
Programs:	Bruker,[1] Olex2,[2] SHELX[3]

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Abstract

$C_{12}H_6Cl_2N_2O_4Cu$, monoclinic, $P2_1/c$ (no. 14), a = 8.3439(5) Å, b = 8.0718(5) Å, c = 20.2384(13) Å, β = 99.650(1)°, V = 1343.78(14) Å^3, Z = 4, $R_{gt}(F)$ = 0.0236, $wR_{ref}(F^2)$ = 0.0633, T = 296 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

6-Chloropyridine-2-carboxylic acid (6.0 mmol) was dissolved in 10 mL of anhydrous methanol. $Cu(CH_3COO)_2{\cdot}H_2O$ (3.0 mmol) dissolved in 10 mL of anhydrous methanol was added dropwise to the above 6-chloropyridine-2-carboxylic acid solution and stirred for 3 h at 60°, cooled and filtered. The filtrate was left for slow evaporation at room temperature. The green block crystals were formed 20 days later. Yield: 32.17 %. Anal. Calcd. For $C_{12}H_6Cl_2N_2O_4Cu$: C, 36.52; H, 2.04; N, 7.10.; found: C, 36.55; H, 2.05; N, 7.15.

2 Experimental details

A suitable crystal was selected and mounted on a Bruker Smart APEX-II CCD. Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

3 Comment

In recent years, metal coordination polymers have garnered significant scientific attention due to their promising applications in materials science and catalysis.[4,5] Among these, carboxylate-based compounds occupy a prominent position in coordination chemistry research, owing to their remarkable structural diversity and versatile physicochemical properties.[6,7] Particularly, pyridine-containing carboxylate ligands have emerged as attractive building blocks due to their unique electronic characteristics and coordination flexibility. In this context, we present the synthesis and structural characterization of a copper-based coordination polymer incorporating 6-chloropyridine-2-carboxylate ligands. As shown in figure, the Cu(II) is five-coordinated in a distorted trigonal bipyramidal environment with three oxygen

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atoms and two nitrogen atoms from three 6-chloropyridine-2-carboxylic acid molecules. The bond angles of O(3)–Cu(1)–O(2), O(3)–Cu(1)–0(1), O(2)–Cu(1)–O(1), N(1)–Cu(1)–O(2), O(2)–Cu(1)–N(2) and N(1)–Cu(1)–N(2) are 129.42(6)°, 112.38(7)°, 118.00(6)°, 97.42(6)°, 92.01(6)° and 169.55(6)°, respectively, which suggest in a distorted trigonal bipyramidal. The Cu(II) centers are interconnected through bridging ligands, propagating along the crystallographic axis to establish an extended one-dimensional coordination polymeric chain.[8] A three-dimensional network is assembled through intermolecular hydrogen bonding and intermolecular π–π interactions. The bond distances of Cu–O are 1.9788(13) and 2.0985(13) Å, which are similar with Refs. 9–11.

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