Hyewon Shin, Jaeun Kang, Kang Min Ok and Junghwan Do*

Crystal structure of catena-poly[(benzylamine-κ¹N)-(sorbato-κ¹O)-(μ₂-sorbato-κ²O,O’)-copper(II), C_{19}H_{23}CuNO₄]

Abstract
C_{19}H_{23}CuNO₄, monoclinic, C2/c (no. 15), a = 16.1601(4) Å, b = 23.3298(7) Å, c = 12.8950(3) Å, β = 128.275(1)°, V = 3816.6(2) Å³, Z = 8, R_{gt}(F) = 0.0620, wR_{ref}(F²) = 0.1251, T = 296(2) K.

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Table 1: Data collection and handling.

| Crystal: | Blue polyhedron |
| Size: | 0.28 × 0.25 × 0.19 mm |
| Wavelength: | Mo Kα radiation (0.71073 Å) |
| μ: | 1.17 mm⁻¹ |
| Diffractometer, scan mode: | Bruker P4, ω |
| θ_max, completeness: | 28.3°, >99% |
| N(hkl)measured, N(hkl)unique, R_{int}: | 24932, 4722, 0.145 |
| Criterion for I_{obs}, N(hkl)_{gt}: | I_{obs} > 2σ(I_{obs}), 2646 |
| N(param)refined: | 228 |
| Programs: | Bruker [1], SHELX [2,3], Diamond [4] |

The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.
The mixture of CuCl (0.030 g, 0.3 mmol), benzylamine (0.033 mL, 0.3 mmol), sorbic acid (0.034 g, 0.3 mmol) in ethanol (1.0 mL) was sealed under vacuum in a Pyrex tube and heated to 70 °C for 68 h, then cooled to room temperature at 20 °C/h. The pH before the reaction was 6 and it remained unchanged after the reaction. The blue polyhedral crystals of the title compound were recovered by vacuum filtration. The product is stable in air.

2 Experimental details

All hydrogen atoms were placed in calculated positions and refined as riding model, and their positions and isotropic displacement parameters were refined. The $U_{iso}$ value of the H atoms in sorbate and benzylamine were set to 1.2 $U_{eq}$ except for the terminal methyl group (1.5 $U_{eq}$) in sorbate.

3 Comment

Many copper(II) complexes have been studied because of their interesting structural features followed by the metal center being able to adopt various coordination geometries such as square planar, square pyramidal, trigonal bi- pyramidal, and octahedral [5]. Specially, copper(II) carboxylates containing nitrogen donor ligands have been extensively studied due to their importance in biology and magnetism [6–9]. In this study we report a 1D copper(II) coordination polymer containing monocarboxylic sorbate anion and benzylamine molecule.

One unique copper atom is coordinated by each one oxygen atoms of three sorbate anions (d(Cu–O) = 1.954(3), 1.958(2), 1.961(2) Å) and one nitrogen atom of benzylamine (d(Cu–N) = 2.001(3) Å) to form a square planar geometry. An additional sorbate oxygen atom is weakly coordinated to Cu in an apical position (d(Cu–O) = 2.409(2) Å), completing the slightly distorted square pyramidal arrangement, as evidenced by the $\tau$ value (angular structure parameter) of 0.02 [10]. The bond valence sum (BVS) calculation for Cu gives a value of +2.024 indicating an oxidation state of +2 [11]. The CuNO$_4$ square pyramids share a common edge of weakly bonded oxygen (O3) atoms to form Cu$_2$NO$_4$ dimeric units with the Cu···Cu distance of about 3.38 Å. The dinuclear Cu(II) unit is positioned around a center of inversion. The dimers are connected to each other by sorbate anions, forming a neutral Cu(benzylamine) (sorbate)$_2$ chain in the [011] direction. The chains are further stabilized by the presence of intra-chain hydrogen bonds between the NH$_2$ of benzylamine and non-coordinated carboxylate O atom [d(NH···O4) = 2.788(4) Å] or the coordinated carboxylate O atom [d(NH···O3) = 2.727(4) Å]. That is, of the two independent sorbates, only one sorbate weakly coordinated with Cu

### 1 Source of material

The mixture of CuCl (0.030 g, 0.3 mmol), benzylamine (0.033 mL, 0.3 mmol), sorbic acid (0.034 g, 0.3 mmol) in ethanol (1.0 mL) was sealed under vacuum in a Pyrex tube and heated to 70 °C for 68 h, then cooled to room temperature at 20 °C/h. The pH before the reaction was 6 and it remained unchanged after the reaction. The blue polyhedral crystals of the title compound were recovered by vacuum filtration. The product is stable in air.
is involved in the hydrogen bonds. Adjacent chains are arranged so that the alkyl group of sorbates are partially interdigitated. The interchain distance between the sorbate groups is >3.78 Å, suggesting that van der Waals interactions predominate with only weak π–π stacking.

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References

1. Bruker. SAINT, APEX2; Bruker Inc.: Madison, WI, USA, 2016.