Crystal structure of catena-poly[aqua-(μ₂-1,4-diazabicyclo[2.2.2]octane-k²N: N’)-bis(sorbato-k¹O)-copper(II), C₁₈H₂₈CuN₂O₅

Abstract

C₁₈H₂₈CuN₂O₅, orthorhombic, Pmmn (no. 59), a = 6.8107(1) Å, b = 24.3351(5) Å, c = 6.0304(1) Å, V = 999.47(3) Å³, Z = 2, R(gt) = 0.0266, wR(ref)(F²) = 0.0676, T = 296(2) K.

CCDC no.: 2326688

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.

Table 1: Data collection and handling.

<table>
<thead>
<tr>
<th>Crystal:</th>
<th>Blue polyhedra</th>
</tr>
</thead>
<tbody>
<tr>
<td>Size:</td>
<td>0.32 × 0.27 × 0.26 mm</td>
</tr>
<tr>
<td>Wavelength:</td>
<td>MoKα radiation (0.71073 Å)</td>
</tr>
<tr>
<td>μ:</td>
<td>1.12 mm⁻¹</td>
</tr>
<tr>
<td>Diffractometer, scan mode:</td>
<td>Bruker P4, ω</td>
</tr>
<tr>
<td>θmax, completeness:</td>
<td>28.3°, &gt;99 %</td>
</tr>
<tr>
<td>N(hkl)measured−N(hkl)unique−Rint:</td>
<td>13,210, 1368, 0.042</td>
</tr>
<tr>
<td>Criterion for Iobs−N(hkl):</td>
<td>Iobs &gt; 2σ(Iobs), 1326</td>
</tr>
<tr>
<td>N(param)refined:</td>
<td>82</td>
</tr>
<tr>
<td>Programs:</td>
<td>Bruker [1], SHELX [2, 3], Diamond [4]</td>
</tr>
</tbody>
</table>

1 Source of material

The mixture of CuCl₂ (0.040 g, 0.3 mmol), dabco (1,4-diazabicyclo[2.2.2]octane; 0.102 g, 1.2 mmol), sorbic acid (0.102 g, 1.2 mmol) in ethanol (1.0 mL) was sealed under vacuum in a Pyrex tube and heated to 140 °C for 68 h, then cooled to room temperature at 20 °C/h. The pH before and after the reaction were 7 and 6, respectively. The blue polyhedral crystals of the title compound were recovered by vacuum filtration. The product is stable in air.

2 Experimental details

Hydrogen atoms were placed in calculated positions and refined as riding model, and their positions and isotropic displacement parameters were refined. The Uiso value of the H atoms in sorbate and dabco were set to 1.2Ueq except for the terminal methyl group (1.5Ueq) in sorbate. The H atoms in water molecules were located in difference Fourier maps, and their positions and isotropic displacement parameters were refined.

3 Comment

Carboxylate compounds are among the most well-represented and are probably one of the most studied classes of coordination chemistry because of their structural

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diversity and numerous useful physical features. However, sorbate complexes are limited in number and only few examples are known so far [5–8]. In this study we report a 1D copper coordination polymer containing sorbate anions and dabco molecules.

One unique copper atom is coordinated by two oxygen atoms and two nitrogen atoms from each two symmetry related sorbate and dabco ligands (d(Cu–O) = 1.928(1) Å, d(Cu–N) = 2.099(2) Å) in trans-configuration to form a square planar geometry. Additionally, one water molecule in an axial position (d(Cu–O) = 2.23(2) Å) completes the slightly distorted square pyramidal environment of Cu1 [9]. The bond valence sum (BVS) calculation for Cu gives a value of +2.01 indicating an oxidation state of +2. The Cu$_2$O$_3$ square pyramidal unit is linked to each other through dabco molecules, forming a neutral CuH$_2$O(dabco)(sorbate)$_2$ chain along the a-axis. Adjacent chains are shifted axially by 1/2a, so that the sorbate groups are interdigitated. The interchain distance between the sorbate groups is >3.93 Å, suggesting that van der Waals interactions predominate with only weak π–π stacking. Furthermore, the chains are stabilized by the presence of interchain hydrogen bonds between the water molecule and the uncoordinated carboxylate oxygen atoms [d(OH⋯O) = 2.660(2) Å] along the c-axis, which results in forming layers on the ac-plane.

**Author contributions:** All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

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

**References**