Crystal structure of \textit{catena-poly}[(\mu_2 \text{-methanolato-} \kappa^2 O: O) - (\mu_2 - 1 -(2 \text{-methyl-} 1H\text{-benzo[d]} \text{imidazol-1-yl)]) \text{-} 1H\text{-benzo[d][1,2,3]triazole-} \kappa^2 N:N')\text{-}(\text{thiocyanato-} \kappa^1 N) \text{copper(II)}] 0.25 hydrate, \textit{C}_{17}\text{H}_{16}\text{CuN}_6\text{OS} \cdot 0.5\text{H}_2\text{O}

Table 1: Data collection and handling.

<table>
<thead>
<tr>
<th>Crystal:</th>
<th>Blue prism</th>
</tr>
</thead>
<tbody>
<tr>
<td>Size</td>
<td>0.18 \times 0.16 \times 0.10 mm</td>
</tr>
<tr>
<td>Wavelength:</td>
<td>Cu K\alpha radiation (1.54184 Å)</td>
</tr>
<tr>
<td>(\mu):</td>
<td>2.93 mm(^{-1})</td>
</tr>
<tr>
<td>Diffractometer, scan mode:</td>
<td>Xcalibur, (\theta)</td>
</tr>
<tr>
<td>(\theta_{\text{max}}):</td>
<td>67.1°, &gt;99%</td>
</tr>
<tr>
<td>(N(hk\ell)<em>{\text{measured}} / N(hk\ell)</em>{\text{unique}} / R_{int}):</td>
<td>7722, 3249, 0.031</td>
</tr>
<tr>
<td>Criterion for (I_{\text{obs}} &gt; \sigma(I_{\text{obs}})):</td>
<td>(I_{\text{obs}} &gt; 2 \sigma(I_{\text{obs}})), 2577</td>
</tr>
<tr>
<td>Programs:</td>
<td>CrysAlis\textsuperscript{PRO} [1], SHELX [2], Diamond [3]</td>
</tr>
</tbody>
</table>

Source of material

All starting materials are commercially available without further purification. 1-\{(2-Methyl-1H-benzoimidazol-1-yl)\text{-}1H-benzotriazole (mbmb) was prepared according to the literature method [4]. The ligand mbmb (0.02 mmol, 0.0053 g) in methanol (6 mL) was added dropwise to an aqueous solution (6 mL) of Cu(CH\text{3COO})\text{2} (0.02 mmol, 0.0040 g). Then an aqueous solution (2 mL) of KSCN (0.02 mmol, 0.0019 g) was added dropwise. The resulting solution was allowed to stand at room temperature. After three weeks blue crystals were obtained.

Experimental details

H atoms were placed in their geometricaly idealized positions and constrained to ride on their parent atoms.

Comment

\(N\)-Heterocyclic compounds are used as important ligands in coordination chemistry and most of these complexes have excellent activity such as anti-cancer activity, anti-
bacterial activity and so forth [5–8]. Especially benzimidazole and benzotriazole compounds are widely used as ligands. Imidazole is a N-containing heterocycle with multiple biological activities. As a pharmaceutical intermediate, imidazole compounds can be used in the production of anti-cancer drugs, anti-fungal drugs and anti-diabetic drugs [9–11]. Benzotriazole, as a typical N-donor ligand, easily binds to DNA, enzymes and receptors in the body through hydrogen bonding, π–π interaction and coordination bonding [12–14].

X-ray crystallographic analysis reveals that the compound centered on binuclear copper is a one-dimensional chain structure, which crystallizes in the monoclinic space group P21/c. As shown in Figure 1, each Cu(II) ion is five-coordinated by two nitrogen donors arising from two mmmb ligands, one nitrogen atoms from a thiocyanate and two oxygen atoms from two coordinated methanoo ligands in a distorted pyramid geometry (with the Cu1–N1 bond length of 2.023(2) Å, the Cu1–N5(1) bond length of 2.425(3) Å, the Cu1–N6 bond length of 1.937(3) Å, and the Cu1–O1 bond length of 1.938(18) Å, the Cu1–O1' bond length of 1.922(19) Å, the symmetry code: \(i = 1-x, 1-y, -z\); \(i1 = -1-x, 1-y, 1-z\); \(i2 = x, y, -1+z\). The bond angles around Cu(II) ion range from 76.63(8) to 169.57(12°). In each mmmb ligand, the dihedral angle between benzotriazole and benzimidazole is 75.6176(1°). Due to the existence of guest water molecules, there are O–H–S hydrogen bonds between guest water molecules and SCN- groups. The geometric parameters are all in the expected ranges [15, 16].

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

References


15. Lan, H.-H Crystal structure of catena-poly(bis(μ2-1,3-di(4H-1,2,4-triazol-4-yl)benzene-κN:N′)-bis(thiocyanato-κN)cobalt(II), C22H16CoN14S2. Z. Kristallogr. NCS 2019, 234, 37–38.