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Crystal structure of *catena*-poly[(μ_2 -methanolato- $\kappa^2 O:O$)-(μ_2 -1-((2-methyl-1H-benzo[d]imidazol-1-yl)methyl)-1H-benzo[d][1,2,3]triazole- $\kappa^2 N:N'$)-(thiocyanato- $\kappa^1 N$)copper(II)] 0.25 hydrate, $C_{17}H_{16}CuN_6OS \cdot 0.5H_2O$

Table 1: Data collection and handling.

Crystal:	Blue prism
Size	0.18 × 0.16 × 0.10 mm
Wavelength:	Cu K α radiation (1.54184 Å)
μ :	2.93 mm ⁻¹
Diffractometer, scan mode:	Xcalibur, ω
$\theta_{\max}$, completeness:	67.1°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	7722, 3249, 0.031
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2577
$N(\text{param})_{\text{refined}}$:	251
Programs:	CrysAlis ^{PRO} [1], SHELX [2], Diamond [3]

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Abstract

$C_{17}H_{16}CuN_6OS \cdot 0.5H_2O$, monoclinic, $P2_1/c$ (no. 14), $a = 10.3523(4)$ Å, $b = 18.2609(9)$ Å, $c = 9.9688(4)$ Å, $\beta = 103.918(4)^\circ$, $Z = 4$, $V = 1829.21(13)$ Å³, $R_{\text{gt}}(F) = 0.0409$, $wR_{\text{ref}}(F^2) = 0.1099$, $T = 291(2)$ K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

All starting materials are commercially available without further purification. 1-[(2-Methyl-1H-benzimidazol-1-yl)methyl]-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 $Cu(CH_3COO)_2$ (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 geometrically 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-

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$).

Atom	x	y	z	U_{iso}^*/U_{eq}
Cu1	0.52872 (4)	0.55818 (2)	0.11152 (4)	0.04380 (15)
S1 ^a	0.7782 (5)	0.7631 (4)	0.2780 (8)	0.0789 (17)
S1A ^b	0.751 (3)	0.7689 (9)	0.2691 (16)	0.115 (3)
O1	0.59522 (18)	0.51885 (12)	−0.0396 (2)	0.0453 (5)
N1	0.4114 (2)	0.60404 (15)	0.2240 (2)	0.0456 (6)
N2	0.3295 (2)	0.65816 (16)	0.3851 (2)	0.0504 (6)
N3	0.2833 (2)	0.62017 (17)	0.5996 (3)	0.0543 (7)
N4	0.3813 (3)	0.57356 (18)	0.6635 (3)	0.0592 (7)
N5	0.3294 (3)	0.52150 (19)	0.7209 (3)	0.0603 (7)
N6	0.6497 (3)	0.64058 (19)	0.1491 (4)	0.0719 (9)
C1	0.2052 (3)	0.61840 (19)	0.0305 (3)	0.0534 (8)
H1	0.239616	0.596029	−0.037258	0.064*
C2	0.0769 (3)	0.6456 (2)	0.0012 (3)	0.0607 (9)
H2	0.023743	0.641150	−0.088010	0.073*
C3	0.0254 (3)	0.6795 (2)	0.1014 (4)	0.0590 (8)
H3	−0.061402	0.697173	0.077670	0.071*
C4	0.1002 (3)	0.6876 (2)	0.2366 (3)	0.0573 (8)
H4	0.066284	0.710609	0.304029	0.069*
C5	0.2281 (3)	0.65941 (18)	0.2648 (3)	0.0465 (7)
C6	0.2805 (3)	0.62583 (17)	0.1650 (3)	0.0446 (6)
C7	0.4375 (3)	0.62442 (18)	0.3541 (3)	0.0472 (7)
C8	0.5676 (3)	0.6155 (3)	0.4562 (3)	0.0657 (10)
H8A	0.630522	0.593439	0.411788	0.099*
H8B	0.556259	0.584779	0.530624	0.099*
H8C	0.599917	0.662631	0.491971	0.099*
C9	0.3182 (3)	0.6800 (2)	0.5219 (3)	0.0563 (8)
H9A	0.402354	0.700577	0.572165	0.068*
H9B	0.251089	0.717983	0.512773	0.068*
C10	0.1625 (3)	0.5958 (2)	0.6172 (3)	0.0527 (8)
C11	0.1940 (3)	0.5320 (2)	0.6956 (3)	0.0524 (8)
C12	0.0959 (3)	0.4913 (2)	0.7360 (4)	0.0649 (9)
H12	0.116247	0.448510	0.787283	0.078*
C13	−0.0313 (4)	0.5171 (3)	0.6969 (5)	0.0762 (12)
H13	−0.099016	0.491644	0.723167	0.091*
C14	−0.0625 (3)	0.5811 (3)	0.6182 (5)	0.0784 (13)
H14	−0.150612	0.596563	0.593350	0.094*
C15	0.0320 (3)	0.6217 (2)	0.5765 (4)	0.0662 (10)
H15	0.010563	0.664070	0.524096	0.079*
C16	0.6968 (3)	0.6937 (2)	0.1992 (4)	0.0557 (8)
C17	0.6799 (3)	0.5558 (2)	−0.1089 (4)	0.0559 (8)
H17A	0.672018	0.607646	−0.097603	0.084*
H17B	0.655083	0.543743	−0.205447	0.084*
H17C	0.770320	0.540994	−0.070774	0.084*
O2 ^c	0.460 (2)	0.7015 (15)	0.859 (3)	0.190 (10)*
H2A ^c	0.483546	0.744822	0.844859	0.285*
H2B ^c	0.521016	0.671682	0.851499	0.285*

^a Occupancy: 0.61(5), ^bOccupancy: 0.39(5), ^cOccupancy: 0.25.

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 $P2_1/c$. As shown in Figure 1, each Cu(II) ion is five-coordinated by two nitrogen donors arising from two mbmb ligands, one nitrogen atoms from a thiocyanate and two oxygen atoms from two coordinated methanoato ligands in a distorted pyramid geometry (with the Cu1–N1 bond length of 2.023(2) Å, the Cu1–N5ⁱⁱ bond length of 2.425(3) Å, the Cu1–N6 bond length of 1.937(3) Å, and the Cu1–O1 bond length of 1.9381(18) Å, the Cu1–O1ⁱ bond length of 1.9222(19) Å, symmetry code: i = 1–x, 1–y, –z; ii = 1–x, 1–y, 1–z; iii = x, y, –1+z). The bond angles around Cu(II) ion range from 76.63(8) to 169.57(12)°. In each mbmb ligand, the dihedral angle between benzotriazole and benzimidazole is 75.617(62)°. 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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