Bo Li*, Zhen-Zhen Shi, Xiao-Jing Xing and Hui-Tao Fan

Crystal structure of *catena*-poly[aqua-bis(formato- κ^1O)-(μ_2 -1,1'-(oxybis(1,4-phenylene))-bis(1*H*-1,2,4-triazole)- $\kappa^2N:N'$)copper(II)]hydrate, $C_{18}H_{16}CuN_6O_6$

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Abstract

$C_{18}H_{16}CuN_6O_6$, monoclinic, $P2_1/c$ (no. 14), $a = 13.669(6)$ Å, $b = 11.311(5)$ Å, $c = 12.763(6)$ Å, $\beta = 93.115(7)^\circ$, $V = 1970.4(15)$ Å³, $Z = 4$, $R_{gt}(F) = 0.0481$, $wR_{ref}(F^2) = 0.1311$, $T = 293(2)$ K.

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A section of the title crystal structure is shown in the figure (Hydrogen atoms are omitted for clarity, $' = -1 + x, y, -1 + z$). Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

A mixture of DMF/H₂O (3/3 mL) containing 1,1'-(oxybis(1,4-phenylene))-bis(1*H*-1,2,4-triazole) (15.2 mg, 0.05 mmol) and Cu(NO₃)₂ (18.7 mg, 0.1 mmol) was placed in a Teflon vessel (12 mL) under autogenous pressure and heated at 100 °C for 72 h and then cooled to room temperature over 24 h. Blue block-shaped crystals were obtained.

Experimental details

Absorption corrections were applied by using multi-scan program. Hydrogen atoms attached to C were treated as riding atoms. The U_{iso} values of the hydrogen atoms of water

*Corresponding author: Bo Li, College of Chemistry and Pharmaceutical Engineering, Nanyang Normal University, Nanyang 473061, China, e-mail: libozzu0107@163.com

Zhen-Zhen Shi, Xiao-Jing Xing and Hui-Tao Fan: College of Chemistry and Pharmaceutical Engineering, Nanyang Normal University, Nanyang 473061, China

Table 1: Data collection and handling.

Crystal:	Blue block
Size:	0.24 × 0.18 × 0.11 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	1.16 mm ⁻¹
Diffractometer, scan mode:	CCD area detector, φ and ω
θ_{max} , completeness:	25.0°, 98%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	6553, 3403, 0.050
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 2412
$N(param)_{refined}$:	280
Programs:	SHELX [1], CrysAlis ^{PRO} [2]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	U_{iso}^*/U_{eq}
Cu1	−0.04160(3)	0.78258(4)	−0.26991(3)	0.03024(19)
C1	0.1681(3)	0.6984(4)	−0.2165(3)	0.0423(11)
H1	0.162555	0.642146	−0.269635	0.051*
C2	0.1308(3)	0.8358(4)	−0.1136(3)	0.0329(9)
H2	0.097566	0.894099	−0.078446	0.039*
C3	0.8058(3)	0.8673(4)	0.5617(3)	0.0324(9)
H3	0.851403	0.895392	0.516244	0.039*
C4	0.7381(3)	0.7943(5)	0.6919(3)	0.0563(14)
H4	0.730546	0.761188	0.757627	0.068*
C5	0.2930(3)	0.8576(4)	−0.0173(3)	0.0311(9)
C6	0.2983(3)	0.9796(4)	−0.0145(3)	0.0400(10)
H6	0.258484	1.024934	−0.060155	0.048*
C7	0.3637(3)	1.0336(4)	0.0573(3)	0.0434(11)
H7	0.366820	1.115683	0.060642	0.052*
C8	0.4245(3)	0.9662(4)	0.1241(3)	0.0377(10)
C9	0.4207(3)	0.8445(4)	0.1193(3)	0.0448(11)
H9	0.462780	0.799114	0.162580	0.054*
C10	0.3534(3)	0.7904(4)	0.0491(3)	0.0403(10)
H10	0.349046	0.708354	0.046921	0.048*
C11	0.5411(3)	0.9805(4)	0.2748(3)	0.0386(10)
C12	0.6388(3)	1.0097(4)	0.2866(3)	0.0465(11)
H12	0.667669	1.054620	0.235651	0.056*
C13	0.6946(3)	0.9718(4)	0.3755(3)	0.0424(11)
H13	0.760252	0.992821	0.384679	0.051*
C14	0.6518(3)	0.9033(3)	0.4490(3)	0.0320(9)
C15	0.5541(3)	0.8733(4)	0.4370(3)	0.0482(12)
H15	0.525289	0.827466	0.487363	0.058*
C16	0.4983(3)	0.9126(4)	0.3480(3)	0.0519(13)
H16	0.432403	0.892470	0.339029	0.062*
C17	0.0594(3)	0.8764(4)	−0.4392(3)	0.0379(10)

Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
H17	0.084782	0.871743	−0.505246	0.045*
C18	−0.1082(3)	0.8718(4)	−0.0807(3)	0.0409(10)
H18	−0.132376	0.863369	−0.014437	0.049*
N1	0.0929(2)	0.7719(3)	−0.1945(2)	0.0330(8)
N2	0.2231(2)	0.8030(3)	−0.0912(2)	0.0337(8)
N3	0.2492(3)	0.7125(3)	−0.1570(3)	0.0461(9)
N4	0.7082(2)	0.8647(3)	0.5413(2)	0.0349(8)
N5	0.6634(3)	0.8164(4)	0.6257(3)	0.0611(13)
N6	0.8271(2)	0.8235(3)	0.6572(2)	0.0355(8)
O1	0.0194(2)	0.7834(2)	−0.40609(19)	0.0367(6)
O2	0.0683(2)	0.9714(3)	−0.3943(2)	0.0520(8)
O3	−0.1048(2)	0.7779(2)	−0.13539(19)	0.0371(6)
O4	−0.0835(2)	0.9717(3)	−0.1048(3)	0.0589(9)
O5	0.4900(2)	1.0307(3)	0.1877(2)	0.0520(8)
O6	−0.0651(2)	0.5884(2)	−0.2931(2)	0.0446(7)
H6A	−0.030684	0.564424	−0.342404	0.053*
H6B	−0.049134	0.553044	−0.238754	0.053*

molecules were set to 1.5*U*_{eq}(O) and the *U*_{iso} values of all other hydrogen atoms were set to 1.2*U*_{eq}(C).

Comment

In recent years, the design and synthesis of coordination polymers based on N-donor ligands have rapidly developed owing to their intriguing structural diversity [3–5]. In addition, the formation of coordination polymers is influenced by the pH value of the reaction, which leads to the completely or partially deprotonated ligands to construct different coordination polymers [6–8]. These N-donor ligands such as triazoles and their derivatives have been used in the synthesis of unique coordination polymers that possess excellent coordination ability. The V-shaped triazole ligand, 1,1'-(oxybis(1,4-phenylene))-bis(1*H*-1,2,4-triazole) (opbt) was used to construct a new coordination polymer. To date, coordination polymers based on this ligand have been limited reported [9].

The asymmetric unit contains one Cu(II) atom, one opbt ligand, two coordinated HCOO[−] ions and one coordinated water molecule. The geometry around the Cu1 atom can be described as a square-pyramidal geometry, and is coordinated by two nitrogen atoms from two different opbt ligands, two oxygen atoms from HCOO[−] ligands, and one oxygen atom from one coordinated water molecule. N1, N6', O1 and O3 atoms comprise the equatorial plane, while the O6

occupy the axial positions. Adjacent copper atoms link opbt ligands to give rise to infinite one-dimensional chain, such chains are further connected through weak non-classical hydrogen bonds.

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