Ying Zhao*, Xiao-Xia Wu and San-Tai Wang

Crystal structure of *catena*-poly[triaqua-(μ_2 -5-methoxy-isophthalato- $\kappa^2 O:O'$)copper(II)], $C_9H_{12}CuO_8$

Table 1: Data collection and handling.

Crystal:	Clear light blue block
Size:	0.18 × 0.14 × 0.08 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	1.95 mm ⁻¹
Diffractometer, scan mode:	APEX, φ and ω
$\theta_{\max}$, completeness:	25.5°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	6795, 2109, 0.099
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1272
$N(\text{param})_{\text{refined}}$:	164
Programs:	SHELX [1], Bruker [2]

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Abstract

[Cu(C₉H₆O₅)(H₂O)₃], monoclinic, $C2/c$ (no. 15), $a = 21.678(13)$ Å, $b = 9.071(6)$ Å, $c = 13.786(9)$ Å, $\beta = 122.738(7)^\circ$, $V = 2280(2)$ Å³, $Z = 8$, $R_{\text{gt}}(F) = 0.0613$, $wR_{\text{ref}}(F^2) = 0.1682$, $T = 296(2)$ K.

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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 5-methoxyisophthalic acid (19.6 mg, 0.1 mmol), a small amount of a base and Cu(OAc)₂·2 H₂O (19.9 mg,

0.1 mmol) were added to water (9 mL) in a 25 mL Teflon-lined autoclave. The mixture was heated at 413 K for 3 days and then slowly cooled down to room temperature. Blue block crystals of the title compound were obtained.

Comment

The construction of novel molecule-based coordination polymers (CPs) with one-dimensional chains to two- or three-dimensional networks has received remarkable attention, not only for understanding the fundamental scientific laws underlying the coordination behaviors of molecular systems, but also for developing applications in many fields [3–7]. Some organic ligands aryl-multicarboxylate are selected as multifunctional ligands, because they can adopt a variety of coordination modes when they react with metal salts to form metal complexes with various multidimensional architectures [8–10].

Each Cu1 center is surrounded by five oxygen atoms (Cu(1)–O(1) = 1.924(5), Cu(1)–O(3)#1 = 1.928(4), Cu(1)–O(6) = 1.979(5), Cu(1)–O(8) = 2.011(5), Cu(1)–O(7) = 2.289(5); symmetry codes: #1 $x + 1/2$, $-y + 3/2$, $z + 1/2$) from two different CH₃O-ip ligands and three coordinated water molecules, forming a CuO₅ distorted trigonal bipyramid. Each CH₃O-ip in the title complex adopts a bridging coordination mode to connect two adjacent copper ions to a chain (*cf.* the figure). The one-dimensional chains are then linked by hydrogen bonding to result in a three-dimensional network structure. All water ligands are involved in hydrogen bonding interactions in this framework.

*Corresponding author: Ying Zhao, College of Chemistry and Chemical Engineering, Henan Key Laboratory of Function-Oriented Porous Materials, Luoyang Normal University, Luoyang, Henan 471934, P.R. China, e-mail: zhaoying_909@sina.com

Xiao-Xia Wu and San-Tai Wang: College of Chemistry and Chemical Engineering, Henan Key Laboratory of Function-Oriented Porous Materials, Luoyang Normal University, Luoyang, Henan 471934, P.R. China

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
Cu1	0.21571(4)	0.62617(9)	0.31273(7)	0.0307(3)
O1	0.1269(2)	0.7407(5)	0.2367(4)	0.0391(13)
O2	0.1892(3)	0.9408(6)	0.3315(4)	0.0412(13)
O3	−0.1939(2)	0.9834(5)	−0.1023(4)	0.0352(12)
O4	−0.1425(3)	0.7658(5)	−0.0304(4)	0.0385(13)
O5	0.0120(3)	1.3510(5)	0.1432(5)	0.0457(14)
O6	0.2021(3)	0.5901(5)	0.4416(4)	0.0362(12)
H6A	0.1711	0.6442	0.4444	0.054 [*]
H6B	0.2437	0.5777	0.5036	0.054 [*]
O7	0.1579(3)	0.4161(5)	0.2124(4)	0.0418(13)
H7A	0.1177	0.4036	0.2081	0.063 [*]
H7B	0.1741	0.3919	0.1705	0.063 [*]
O8	0.2327(3)	0.6728(5)	0.1864(4)	0.0388(13)
H8A	0.2525	0.7573	0.1982	0.058 [*]
H8B	0.2586	0.6009	0.1885	0.058 [*]
C1	0.1307(4)	0.8781(8)	0.2585(5)	0.0313(16)
C2	0.0617(3)	0.9645(7)	0.1890(5)	0.0258(15)
C3	0.0641(4)	1.1180(7)	0.1988(5)	0.0287(15)
H3	0.1078	1.1645	0.2523	0.034 [*]
C4	0.0023(4)	1.2004(7)	0.1299(6)	0.0329(17)
C5	−0.0641(4)	1.1343(8)	0.0537(5)	0.0307(16)
H5	−0.1059	1.1910	0.0079	0.037 [*]
C6	−0.0676(3)	0.9795(7)	0.0468(5)	0.0252(15)
C7	−0.0047(4)	0.8976(7)	0.1138(6)	0.0296(16)
H7	−0.0071	0.7953	0.1081	0.035 [*]
C8	−0.1393(4)	0.9039(8)	−0.0343(5)	0.0302(17)
C9	−0.0511(5)	1.4406(9)	0.0828(9)	0.084(4)
H9A	−0.0734	1.4277	0.0013	0.125 [*]
H9B	−0.0375	1.5421	0.1027	0.125 [*]
H9C	−0.0854	1.4130	0.1033	0.125 [*]

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