Wenjun Li and Si Lang Jiu Mai*

Crystal structure of poly[diaqua-(μ_8 -1,1':2',1''-terphenyl-3,3'',4',5'-tetracarboxylato- $\kappa^8 O^1:O_2:O^3:O^4:O^5:O^6:O^7:O^8$)dicopper(II)], $C_{22}H_{14}Cu_2O_{10}$

Table 1: Data collection and handling.

Crystal:	Blue block
Size:	0.28 × 0.26 × 0.14 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	2.02 mm ⁻¹
Diffractometer, scan mode:	Xcalibur, ω
$\theta_{\max}$, completeness:	26.4°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	6566, 2219, 0.044
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1741
$N(\text{param})_{\text{refined}}$:	155
Programs:	CrysAlis ^{PRO} [1], Olex2 [2], SHELX [3]

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.36434(5)	0.53884(4)	0.51534(2)	0.01473(15)
O1	0.3822(3)	0.4180(3)	0.57738(11)	0.0276(7)
O2	0.6056(3)	0.3429(3)	0.54747(10)	0.0267(6)
O3	0.5303(3)	0.1645(2)	0.93535(10)	0.0248(6)
O4	0.2991(3)	0.0977(3)	0.96167(10)	0.0257(6)
O5	0.1285(3)	0.5826(3)	0.53362(15)	0.0440(8)
H5A	0.0726	0.5675	0.5043	0.066*
H5B	0.1184	0.6642	0.5388	0.066*
C1	0.4946(5)	0.3450(3)	0.58138(13)	0.0186(8)
C2	0.4991(4)	0.2538(3)	0.62973(14)	0.0192(8)
C3	0.5795(5)	0.1412(4)	0.62559(16)	0.0311(10)
H3	0.6368	0.1237	0.5935	0.037*
C4	0.5741(6)	0.0540(4)	0.66967(17)	0.0382(12)
H4	0.6278	−0.0226	0.6670	0.046*
C5	0.4895(5)	0.0799(4)	0.71766(15)	0.0291(10)
H5	0.4850	0.0198	0.7466	0.035*
C6	0.4117(4)	0.1948(3)	0.72284(14)	0.0185(8)
C7	0.4164(4)	0.2812(3)	0.67845(14)	0.0168(8)
H7	0.3638	0.3583	0.6812	0.020*
C8	0.3217(4)	0.2223(3)	0.77532(13)	0.0176(8)
C9	0.3895(4)	0.1916(3)	0.82716(13)	0.0174(8)
H9	0.4842	0.1521	0.8273	0.021*
C10	0.3194(4)	0.2185(3)	0.87837(13)	0.0149(7)
C11	0.3884(4)	0.1579(3)	0.93014(14)	0.0171(8)

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Abstract

$C_{22}H_{14}Cu_2O_{10}$, orthorhombic, *Pccn* (no. 56), $a = 8.7989(3)$ Å, $b = 10.4284(3)$ Å, $c = 23.6873(6)$ Å, $V = 2173.51(11)$ Å³, $Z = 8$, $R_{\text{gt}}(F) = 0.0398$, $wR_{\text{ref}}(F^2) = 0.0969$, $T = 293(2)$ K.

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A part of the title coordination polymer 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.

*Corresponding author: Si Lang Jiu Mai, Department of Medical Oncology, Baiyu Country People's Hospital of Sichuan Province, Ganzi, Sichuan, China, e-mail: silang_jiumai66@126.com

Wenjun Li: Department of Obstetrics and Gynecology, Chengdu Tumor Hospital, Chengdu, Sichuan, China

Source of material

A mixture of H_4L ([1,1':2',1''-terphenyl]-3,3'',4',5'-tetracarboxylic acid, 0.1 mmol, 40.6 mg), $Cu(NO_3)_2 \cdot 3 H_2O$

(0.1 mmol, 24 mg), KOH (0.4 mmol, 22.4 mg) and H₂O (10 mL) was placed in a Teflon-lined stainless steel vessel (25 mL), heated to 160 °C for 3 days, and then cooled to room temperature over 24 h. Blue block crystals of the title complex were obtained. Yield 48% based on Cu.

Comment

Studies of metal–organic frameworks (MOFs) or coordination polymers (CPs) are of considerable interest due to their fascinating network topologies and potential applications as functional materials [4–6]. Coordination mode of organic linkers and the geometry of metal cations have a major impact on the topology [7]. Usually, multi-dentate organic ligands like multi-carboxylic acids to extend open frameworks, because these ligands may potentially provide various coordination modes and favor the construction of multi-dimensional coordination polymers. 1,1':2'',1''-terphenyl-3,3''4',5'-tetracarboxylic acid has been shown to be a flexible and big organic ligand [8, 9]. The four carboxyl groups of 1,1':2'',1''-terphenyl-3,3''4',5'-tetracarboxylic acid may be completely or partially deprotonated, inducing various coordination modes and allowing higher dimensionality structures.

The single-crystal X-ray diffraction analysis reveals that the title complex belongs to the orthorhombic space group *Pccn* showing a three-dimensional framework structure. There is one crystallographic independent Cu(II) ion, a half L^{4−} ligand and one coordinated water in the asymmetric unit. The coordination environment of Cu(II) ion is completed by four carboxyl O atoms from four different L^{4−} ligands and one coordinated water molecule. Two symmetry-related Cu(II) ions are held together by four carboxylic groups to afford the well known binuclear paddle-wheel cluster, which

is connected by the L^{4−} ligands to form a three-dimensional framework. This 3D framework is stabilized by the H-bond interaction between H5B and O3 with a distance of 2.014 Å.

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