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The crystal structure of *catena*-poly[chlorido-(μ_2 -1,4-bis(pyridin-3-yl-methoxy)benzene- $\kappa^2 N:N'$)copper(II)], $C_{18}H_{16}ClN_2O_2Cu$

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Abstract

$C_{18}H_{16}ClN_2O_2Cu$, monoclinic, $C2/c$ (no. 15), $a = 23.330(5)$ Å, $b = 7.1347(14)$ Å, $c = 10.328(2)$ Å, $\beta = 108.33(3)^\circ$, $V = 1632.0(6)$ Å³, $Z = 4$, $R_{gt}(F) = 0.0275$, $wR_{ref}(F^2) = 0.0763$, $T = 296(2)$ 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.

Table 1: Data collection and handling.

Crystal:	Green block
Size:	0.30 × 0.20 × 0.10 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	1.52 mm ^{−1}
Diffractometer, scan mode:	Xcalibur, φ and ω
θ_{max} , completeness:	25.5°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	5928, 1518, 0.028
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 1336
$N(param)_{refined}$:	110
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 3]

Source of material

A mixture of $CuCl_2 \cdot 2H_2O$ (0.04 mmol, 7 mg), 1,4-bis(pyridin-3-ylmethoxy)benzene (1,4-bpyb) (0.02 mmol, 6 mg), MeCN/ H_2O (3 mL/2 mL), was dissolved in 9 mL H_2O . Then the solution was heated in a 23 mL Teflon-lined autoclave under autogenous pressure at 403 K for three days. After cooling to room temperature green crystals suitable for X-ray diffraction analysis were collected.

Experimental details

Hydrogen atoms were positioned in accord with the chemical surrounding. Their U_{iso} values were set to $1.2U_{eq}$ of the parent atoms.

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

Atom	x	y	z	<i>U</i> _{iso} */ <i>U</i> _{eq}
Cu1	0.5000	0.21986(6)	0.7500	0.04474(17)
Cl1	0.5000	0.54022(12)	0.7500	0.0546(3)
C1	0.56443(10)	−0.0541(3)	0.6415(2)	0.0435(6)
H1	0.5458	−0.1399	0.6832	0.052*
C2	0.60098(12)	−0.1196(3)	0.5706(3)	0.0517(6)
H2	0.6064	−0.2478	0.5631	0.062*
C3	0.62958(10)	0.0057(3)	0.5104(2)	0.0441(6)
H3	0.6549	−0.0370	0.4629	0.053*
C4	0.62047(9)	0.1942(3)	0.5212(2)	0.0337(5)
C5	0.58179(10)	0.2498(3)	0.5921(2)	0.0362(5)
H5	0.5744	0.3772	0.5975	0.043*
C6	0.65002(10)	0.3382(3)	0.4571(2)	0.0391(5)
H6A	0.6725	0.2769	0.4044	0.047*
H6B	0.6196	0.4180	0.3963	0.047*
C7	0.71894(9)	0.5955(3)	0.5266(2)	0.0308(4)
C8	0.75543(9)	0.7016(3)	0.6323(2)	0.0333(5)
H8	0.7592	0.6691	0.7218	0.040*
C9	0.78655(9)	0.8557(3)	0.6075(2)	0.0325(5)
H9	0.8109	0.9260	0.6797	0.039*
N1	0.55450(8)	0.1291(3)	0.65311(19)	0.0382(4)
O1	0.68951(7)	0.4469(2)	0.56254(14)	0.0420(4)

Comment

Organic ligands such as 4,4'-bis(pyrid-4-yl)biphenyl, have great influence on the cooresponding coordination polymers and MOFs [4–6]. Flexible *N*-donor ligands can result in gauche and anti conformations in coordination to meet the requirements of the coordination of different metal ions in the assembly process. The organic ligand 1,4-bis(pyridin-3-ylmethoxy)benzene is known to serve as bridging ligand [7–9].

In the title complex, there are one half of a Cu(II) ion, one half of a 1,4-bpyb ligand, and one half of a chlorine in the asymmetric unit. The copper atom Cu1 is three-coordinated by two N atoms from the 1,4-bpyb ligands (see the figure). The Cu—Cl bond length is 2.2856(11) Å; and the Cu—N

bond length is 1.9589(18) Å, respectively. The bond angle of N—Cu—N is 141.40(11)°.

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References

1. Agilent Technologies: CrysAlis^{PRO} Software system, version 1.171.35.15. Agilent Technologies UK Ltd, Oxford, UK (2011).
2. Sheldrick, G. M.: SHELXT – Integrated space-group and crystal-structure determination. *Acta Crystallogr.* **A71** (2015) 3–8.
3. Sheldrick, G. M.: Crystal structure refinement with SHELXL. *Acta Crystallogr.* **C71** (2015) 3–8.
4. Li, S. H.; Hu, X. Z.; Zhao, Y.: Crystal structure of *catena*-poly [diaqua-μ₂-4,4'-biphenyl-4,4'-diylbipyridine-κ²*N:N'*-bis(5-carboxy-2,6-dimethylpyridine-3-carboxylato-κ*O*)nickel(II)] dihydrate. *Z. Kristallogr. NCS* **231** (2016) 157–159.
5. Chen, S. J.; Li, S. H.; Wang, W. H.; Long, Y. F.; Zhang, W. L.; Wang, T.; Xu, Y. L.: Crystal structure of poly[aqua-μ₂-4,4'-bis (pyrid-4-yl) biphenyl-κ²*N:N'*]-μ₄-4'-methyl-[1,1'-biphenyl]-3,5-dicarboxylato-κ⁴*O:O':O'':O'''*)manganese(II)]. *Z. Kristallogr. NCS* **234** (2019) 373–375.
6. Zhao, Y.; Hu, X. Z.; Zhang, R.: Crystal structure of poly [dibromido-(μ₂-4,4'-bis-(pyrid-4-yl)biphenyl-κ²*N:N'*)lead(II)]. *Z. Kristallogr. NCS* **231** (2016) 191–192.
7. Li, S. H.; Zhao, Y.: Synthesis and crystal structure of a new three-dimensional Co(II) coordination polymer based on 3,3', 4,5'-biphenyl tetracarboxylic acid and 4,4'-bipyridine. *Inorg. Nano-Met. Chem.* **47** (2017) 256–259.
8. Song, W.; Xu, X. L.; Yang, Y. J.; Li, S. H.: Synthesis and crystal structure of *catena*-poly[bis(2-(2-(2,6-dichlorophenyl) amino)phenyl)acetato-κ*O*;κ²*O',O''*)-(μ₂-1,4-di(pyridin-4-yl) benzene-κ²*N:N'*)zinc(II)]. *Z. Kristallogr. NCS* **233** (2018) 399–401.
9. Li, S. H.; Li, X. L.: A cadmium complex based on 5-methylisophthalic acid and 1,6-bis(imidazol-1-yl)hexane: synthesis, crystal structure, and photoluminescence properties. *Synth. React. Inorg. Met.-Org. Nano-Met. Chem.* **43** (2013) 710–713.