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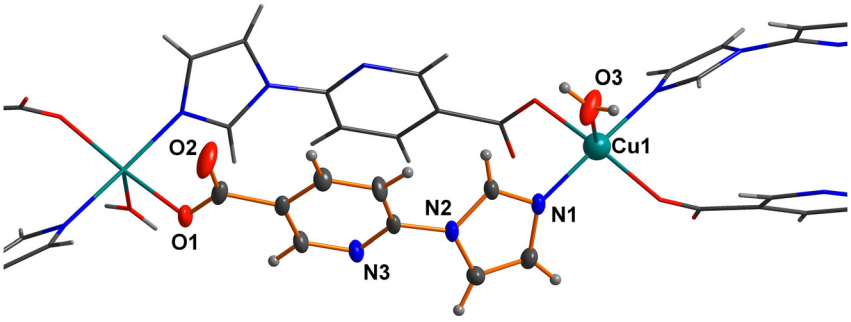
Crystal structure of *catena*-poly[aqua-bis[μ_2-6-(1*H*-imidazol-1-yl)nicotinato-κ^2 *N*,*O*]copper(II)], $C_{18}H_{14}N_6O_5Cu$



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Abstract

$C_{18}H_{14}N_6O_5Cu$, monoclinic, *C*2/*c* (no. 15), a = 14.1337(5) Å, b = 5.8568(2) Å, c = 21.2295(6) Å, β = 105.074(3)°, V = 1696.87(10) Å^3, Z = 4, $R_{gt}(F)$ = 0.0239, $wR_{ref}(F^2)$ = 0.0603, T = 293 K.

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A section of the polymeric title crystal structure 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:	Blue block
Size:	0.34 × 0.30 × 0.29 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	1.34 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max}, completeness:	25.0°, 99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	4567, 1483, 0.015
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 1427
$N(param)_{refined}$:	141
Programs:	CrysAlis^{PRO} [1], SHELX [2, 3], Olex2 [4]

Source of material

All chemicals were purchased and used without further purification. The title compound was prepared under the hydrothermal conditions by the following procedure: a mixture of 6-(1*H*-imidazol-1-yl)nicotinic acid (18.9 mg, 0.1 mmol), $Cu(OAc)_2{\cdot}H_2O$ (20 mg, 0.1 mmol), and 8 mL deionized water was sealed in a 25 mL Teflon-lined stainless steel vessel and heated at 413 K for four days under autogenous pressure, followed by cooling to room temperature, blue block crystals of were obtained (yield: 53% based on Cu).

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Comment

In recent years, coordination polymers have received much attention due to their interesting photophysical properties and potential application [5–7]. At present, the rational design of coordination polymers is still a challenging task [8–10]. In the synthesis of coordination polymers, N-donor

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Cu1	1.0000	0.17199 (6)	0.7500	0.01714 (12)
O1	0.48044 (11)	0.3627 (3)	0.33944 (7)	0.0266 (4)
O2	0.53618 (16)	0.7190 (3)	0.36191 (8)	0.0447 (5)
O3	1.0000	0.5464 (4)	0.7500	0.0409 (7)
N1	0.85687 (13)	0.1610 (3)	0.70912 (8)	0.0208 (4)
N2	0.72519 (13)	0.2227 (3)	0.62936 (8)	0.0189 (4)
N3	0.61491 (14)	0.1563 (3)	0.52867 (8)	0.0224 (4)
C1	0.52573 (16)	0.5190 (4)	0.37711 (10)	0.0230 (5)
C2	0.57435 (15)	0.4484 (4)	0.44661 (9)	0.0177 (4)
C3	0.56735 (16)	0.2287 (4)	0.46858 (10)	0.0216 (5)
H3A	0.5277	0.1252	0.4404	0.026*
C4	0.66921 (15)	0.3091 (4)	0.56785 (9)	0.0179 (4)
C5	0.67831 (16)	0.5345 (4)	0.55206 (10)	0.0235 (5)
H5	0.7154	0.6364	0.5822	0.028*
C6	0.63028 (16)	0.6034 (4)	0.48978 (10)	0.0232 (5)
H6	0.6355	0.7537	0.4769	0.028*
C7	0.70613 (16)	0.0311 (4)	0.66219 (10)	0.0238 (5)
H7	0.6491	−0.0558	0.6526	0.029*
C8	0.78793 (16)	−0.0033 (4)	0.71122 (10)	0.0244 (5)
H8	0.7963	−0.1204	0.7418	0.029*
C9	0.81661 (15)	0.2944 (4)	0.65976 (9)	0.0197 (5)
H9	0.8469	0.4214	0.6473	0.024*
H3	0.995 (3)	0.628 (5)	0.7185 (14)	0.062 (11)*

spacer ligands have been widely used due to their molecular geometry and strong coordination ability [11, 12]. However, to date, organic ligands containing both imidazole and pyridine functional groups are rarely involved. The rigid 6-(1*H*-imidazol-1-yl)nicotinate ligand containing a nicotinic and an imidazole moiety may show versatile coordination modes, which makes it a useful bridge to construct coordination polymers.

Single crystal X-ray structural analysis shows that the compound is a one-dimensional chain structure and crystallizes in the monoclinic space group *C*2/*c*. The asymmetric unit of the title crystal structure consists of one half of a Cu^{2+} ion, one fully deprotonated 6-(1*H*-imidazol-1-yl)nicotinate anion, and one half a coordinated water molecule. The five-coordinated Cu1 atom is in a distorted square-pyramidal environment coordinated by two carboxylate oxygen atoms from two different 6-(1*H*-imidazol-1-yl)nicotinate anion, two imidazole nitrogen atoms from two different 6-(1*H*-imidazol-1-yl)nicotinate anion and one coordinated water molecule (see the figure). The Cu–O distances associated with central Cu atoms are 1.9990(14) and 2.193(3) Å. The Cu–N distance is 1.9840(17) Å. The Cu–O/N distances are within the normal ranges [13]. As a result, the adjacent Cu^{2+} ions are connected by 6-(1*H*-imidazol-1-yl)nicotinate anions to form a 1D chain, with a Cu···Cu separation of 11.1549(4) Å.

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References

1. Agilent Technologies. CrysAlis^{PRO} Software system (version 1.171.38.41r); Agilent Technologies UK Ltd: Oxford, UK, 2015.
2. Sheldrick G. M. *SHELXTL* – integrated space-group and crystal-structure determination. *Acta Crystallogr.* 2015, *A71*, 3–8.
3. Sheldrick G. M. Crystal structure refinement with SHELXL. *Acta Crystallogr.* 2015, *C71*, 3–8.
4. Dolomanov O. V., Bourhis L. J., Gildea R. J., Howard J. A. K., Puschmann H. OLEX2: a complete structure solution, refinement and analysis program. *J. Appl. Crystallogr.* 2009, *42*, 339–341.
5. Cook T. R., Zheng Y. R., Stang P. J. Metal-organic frameworks and self-assembled supramolecular coordination complexes: comparing and contrasting the design, synthesis, and functionality of metal-organic materials. *Chem. Rev.* 2012, *113*, 734–777.
6. Yang L., Tan X., Wang Z., Zhang X. Supramolecular polymers: historical development, preparation, characterization, and functions. *Chem. Rev.* 2015, *115*, 7196–7239.
7. Vittal J. J. Supramolecular structural transformations involving coordination polymers in the solid state. *Coord. Chem. Rev.* 2007, *251*, 1781–1795.
8. Roesky H. W., Andruh M. The interplay of coordinative, hydrogen bonding and π–π stacking interactions in sustaining supramolecular solid-state architectures. A study case of bis(4-pyridyl)- and bis(4-pyridyl-*N*-oxide)tectons. *Coord. Chem. Rev.* 2003, *236*, 91–119.
9. Sun Y., Sun W. Influence of temperature on metal-organic frameworks. *Chin. Chem. Lett.* 2014, *25*, 823–828.
10. Li J., Li R., Li M., Shao M., He X. Enhancing water stability in Co(II) coordination polymers from their structural transformation by temperature-controlling and their dye degradation property. *J. Solid State Chem.* 2021, *298*, 122110.
11. Liu Q., Guo J., Wang Y., Wei J., Chen Y., Hu C. Ionothermal syntheses and characterization of 2-D coordination polymers with 4-(1*H*-imidazol-1-yl)benzoic acid. *J. Coord. Chem.* 2013, *66*, 530–538.
12. Li F., Guo Y. A new 1D ladder-like cadmium(II) coordination polymer based on 4-(1*H*-Imidazol-1-yl)benzoate and chloro ligands: crystal structure and luminescence. *Chin. J. Inorg. Chem.* 2013, *29*, 1527–1538.
13. Li Z.-H. Crystal structure of tetraaqua-bis[6-(1*H*-imidazol-1-yl-κ*N*) nicotinato]zinc(II), $C_{18}H_{20}N_6O_8Zn$. *Z. Kristallogr. N. Cryst. Struct.* 2018, *233*, 273–274.