Poly[[bis[μ_4-3-(2-carboxylatophenyl)propionato]-{N-[2-(pyridine-3-amido)ethyl]nicotinamide}-dicopper(II)] pentahydrate]

Gabrielle J. Gaskin and Robert L. LaDuca*

E-35 Holmes Hall, Michigan State University, Lyman Briggs College, 919 E. Shaw Lane, East Lansing, MI 48825, USA. *Correspondence e-mail: laduca@msu.edu

In the title compound, $\{[Cu_2(C_{10}H_8O_4)_2(C_{14}H_{14}N_4O_2)]\cdot 5H_2O\}_n$, the Cu^{II} cations are coordinated in a square-pyramidal fashion, with four 3-(2-carboxyphenyl)propionate (cpp) carboxylate O-atom donors in the basal plane, along with an N-atom donor from a N-[2-(pyridin-3-ylamino)ethyl]nicotinamide (pen) ligand in the apical position. $[Cu_2(cpp)_2]_n$ coordination polymer layer motifs with embedded $\{Cu_2(OCO)_4\}$ paddlewheel clusters are thereby constructed. These layer motifs are connected into a three-dimensional $[Cu_2(cpp)_2(pen)]_n$ coordination polymer network by tethering pen ligands. Treating the $\{Cu_2(OCO)_4\}$ paddelwheel clusters as 6-connected nodes reveals an underlying cross-pillared self-penetrated **rob** network with $4^8 6^6 8$ topology. The water molecules of crystallization are held to the coordination polymer network by N—H···O and O—H···O hydrogen-bonding patterns.

3D view	Chemical scheme
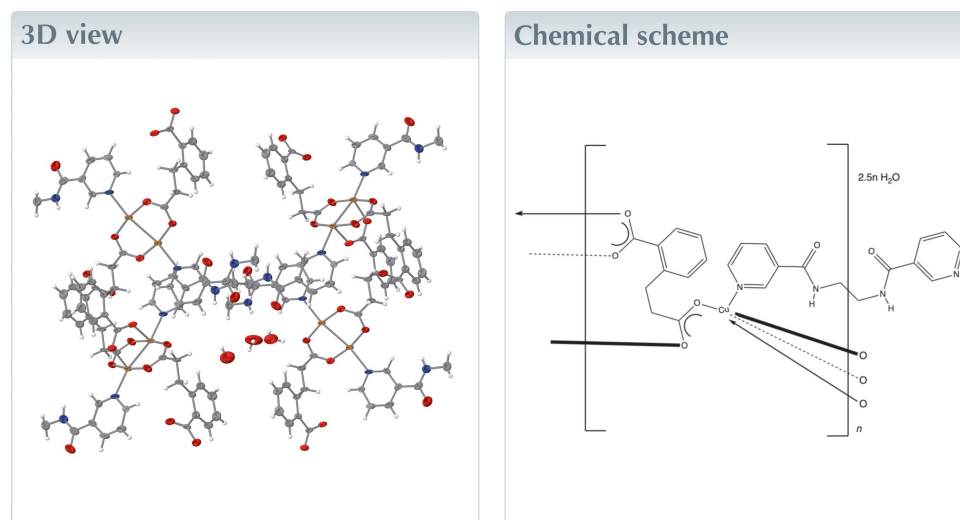
Structure description

The title compound was isolated during an exploratory synthetic effort aiming to produce a copper coordination polymer containing both 3-(2-carboxyphenyl)propionic (cpp) and N-(2-(pyridin-3-ylamino)ethyl)nicotinamide (pen) ligands. The pen ligand has to date seldom been used in coordination polymer chemistry (Wang *et al.*, 2013). Our group has previously reported a racemic cobalt camphorate pen-containing coordination polymer with $4^{12} 6^3$ **pcu** topology (Przybyla *et al.*, 2019)

The asymmetric unit of the title compound contains a divalent copper atom, a fully deprotonated cpp ligand, half of a pen ligand whose central ethylene moiety is sited over a crystallographic inversion center (Wyckoff special position *a*), two water molecules of crystallization located on general positions, and one water molecule of crystallization best

Table 1
Selected geometric parameters (Å, °).

Cu1—O2	1.965 (5)	Cu1—O5^{iii}	1.975 (5)
Cu1—O3^{i}	1.967 (5)	Cu1—N1	2.172 (6)
Cu1—O4^{ii}	1.991 (5)		
O2—Cu1—O3^{i}	168.9 (2)	O3^{i}—Cu1—O5^{iii}	87.1 (2)
O2—Cu1—O4^{ii}	90.1 (2)	O3^{i}—Cu1—N1	97.5 (2)
O2—Cu1—O5^{iii}	91.5 (2)	O4^{ii}—Cu1—N1	87.0 (2)
O2—Cu1—N1	93.6 (2)	O5^{iii}—Cu1—O4^{ii}	168.0 (2)
O3^{i}—Cu1—O4^{ii}	89.0 (2)	O5^{iii}—Cu1—N1	104.8 (2)

Symmetry codes: (i) $-x + \frac{1}{2}, -y + \frac{1}{2}, -z + 1$; (ii) $x, -y + 1, z + \frac{1}{2}$; (iii) $-x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$.

refined at half occupancy and disordered about a crystallographic twofold rotation axis (Wyckoff special position *e*). The copper atoms in the title compound display a {CuNO$_4$} square-pyramidal coordination environment (Fig. 1), with a pyridyl nitrogen donor atom from a pen ligand located in the elongated apical position. Carboxylate oxygen atom donors from four different cpp ligands occupy the basal plane, with the two 'longer-arm' ethyl-carboxylate group oxygen atoms in *trans* position to each other, and the two 'shorter-arm' benzoate carboxylate group oxygen atoms in the other two positions, also *trans* to each other. Bond lengths and angles within the coordination environment in the title compound are listed in Table 1.

The cpp ligands in the title compound connect four copper atoms in an exotetradentate pattern in which each carboxylate oxygen atom binds only to one copper atom. Via four cpp carboxylate groups – two from the longer-arm cpp termini and two from the shorter-arm cpp termini – {Cu$_2$(OCO)$_4$} paddlewheel dimeric units are formed (Fig. 1). These have a through-space Cu···Cu internuclear distance of 2.620 (1) Å, and their centroids are located on crystallographic inversion centers (Wyckoff special position *d*). Each of these dimeric units connects to four others through the full span of the cpp ligands thereby forming [Cu$_2$(cpp)$_2$]$_n$ coordination polymer layers arranged parallel to the *bc* crystal planes (Fig. 2). Parallel [Cu$_2$(cpp)$_2$]$_n$ coordination polymer layers are pillared into a three-dimensional [Cu$_2$(cpp)$_2$(pen)]$_n$ coordination

Figure 2
[Cu$_2$(cpp)$_2$]$_n$ coordination polymer layer in the title compound, featuring {Cu$_2$(OCO)$_4$} paddlewheel clusters. Water molecules of crystallization have been omitted.

polymer network (Fig. 3) by *anti*-conformation ebn ligands that span a Cu···Cu distance of 14.87 (1) Å. The nearest internuclear distance between adjacent [Cu$_2$(cpp)$_2$]$_n$ layers is 12.08 (1) Å, which is too short to be spanned directly by the pen ligands given their conformational constraints. As a result, the three-dimensional [Cu$_2$(cpp)$_2$(pen)]$_n$ network is formed by cross-pillaring of the pen tethers, thereby precluding a much more common straight-pillared 4^{12}6^3 **pcu** topology. Treating

Figure 1
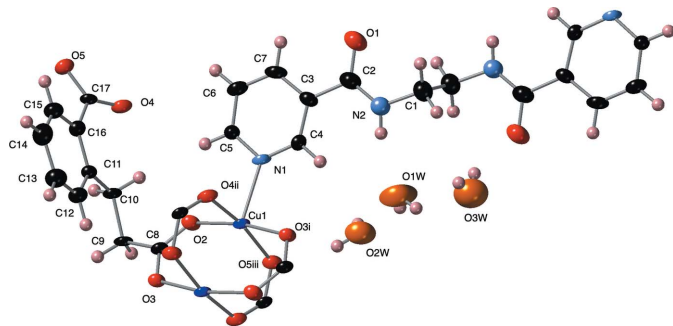Coordination environment in the title compound with full ligand set and complete {Cu$_2$(OCO)$_4$} paddlewheel cluster. Water molecules of crystallization are shown. Displacement ellipsoids are drawn at the 50% probability level. Color code: Cu, dark blue; O in ligands, red; O in water molecules of crystallization, orange; N, light blue; C, black; H, pink. Symmetry codes are as listed in Table 1.
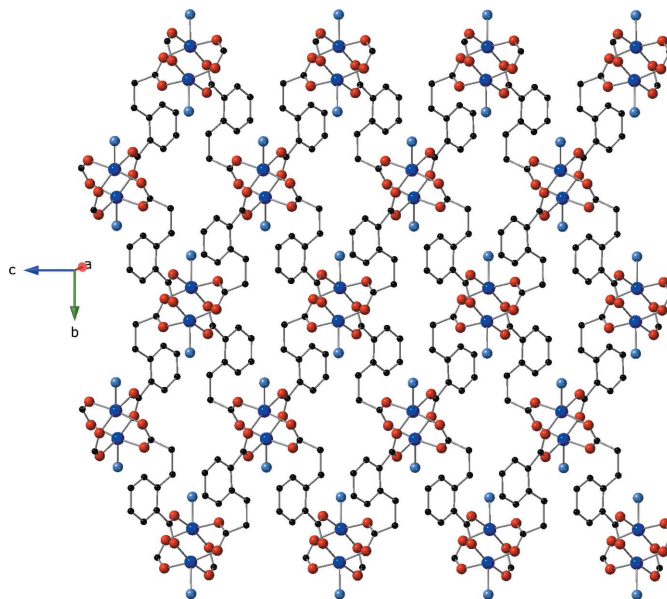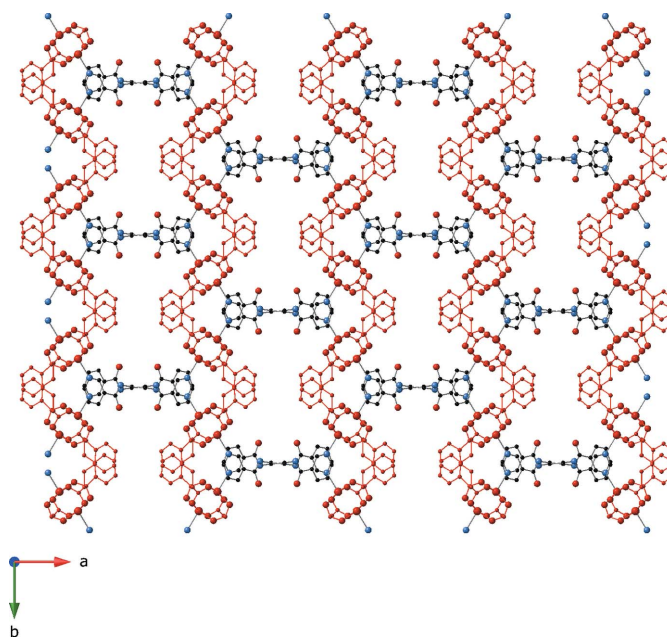

Figure 3
[Cu$_2$(cpp)$_2$(pen)]$_n$ coordination polymer network in the title compound, with [Cu$_2$(cpp)$_2$]$_n$ layers drawn in red

Table 2
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N2—H2$\cdots$O1W	0.87 (2)	2.03 (4)	2.844 (10)	155 (8)
C5—H5$\cdots$O2	0.95	2.50	3.099 (9)	121
C6—H6$\cdots$O3^{iv}	0.95	2.48	3.332 (9)	149
O1W—H1$WA\cdots$O2W	0.85 (2)	2.00 (11)	2.698 (13)	139 (15)
O1W—H1$WB\cdots$O3W	0.85 (2)	2.10 (2)	2.79 (2)	139 (5)
O2W—H2$WA\cdots$O5^{iii}	0.85 (2)	2.09 (2)	2.909 (10)	162 (7)
O2W—H2$WB\cdots$O1^{v}	0.85 (2)	2.06 (2)	2.816 (9)	147 (5)
O3W—H3$WA\cdots$O1^{ii}	0.84 (2)	2.10 (2)	2.917 (19)	162 (9)
O3W—H3$WB\cdots$O1^{vi}	0.84 (2)	2.10 (2)	2.848 (19)	147 (6)

Symmetry codes: (ii) $x, -y+1, z+\frac{1}{2}$; (iii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (iv) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (v) $x, -y+1, z-\frac{1}{2}$; (vi) $-x+1, -y+1, -z+2$.

each {Cu$_2$(OCO)$_4$} paddlewheel dimeric unit as a 6-connected node results in an uncommon self-penetrated, cross-pillared **rob** network with $4^8 6^6 8$ topology when analyzed using the *TOPOS* software (Blatov *et al.*, 2014) (Fig. 4). Discrete D(3) short water molecule chains (Infantes & Motherwell, 2002) positioned along the *c*-axis crystal direction occupy incipient channels comprising 21.8% of the unit cell volume according to *PLATON* (Spek, 2020).

The co-crystallized water molecules are held to the coordination polymer framework by hydrogen-bonding acceptance from the pen N—H groups, and hydrogen-bonding donation to each other. Details regarding the hydrogen bonding in the title compound are listed in Table 2.

Synthesis and crystallization

Cu(NO$_3$)$_2$·2.5 H$_2$O (87 mg, 0.37 mmol), 3-(2-carboxyphenyl)propionic acid (cppH$_2$) (73 mg, 0.37 mmol), *N*-(2-(pyridin-
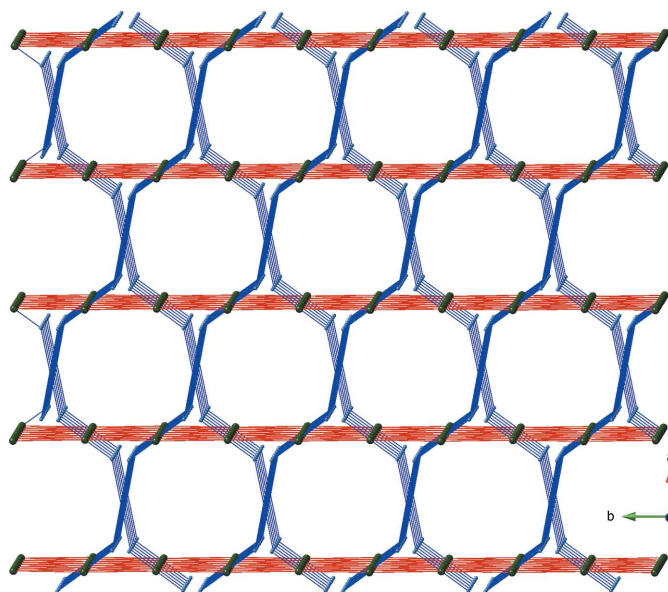

Figure 4
Schematic perspective of the $4^8 6^6 8$ **rob** cross-pillared self-penetrated topology in the title compound. The spheres represent the centroids of the 6-connected {Cu$_2$(OCO)$_4$} paddlewheel clusters. The [Cu$_2$(cpp)$_2$]$_n$ layers are drawn in red, with the cross-pillaring pen ligands drawn in blue.

Table 3
Experimental details.

Crystal data	
Chemical formula	[Cu$_2$(C$_{10}$H$_8$O$_4$)$_2$(C$_{14}$H$_{14}$N$_4$O$_2$)]·5H$_2$O
M_r	871.78
Crystal system, space group	Monoclinic, $C2/c$
Temperature (K)	173
a, b, c (Å)	27.558 (10), 14.873 (5), 9.146 (3)
β (°)	98.396 (4)
V (Å^3)	3709 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.22
Crystal size (mm)	0.28 × 0.16 × 0.11
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.560, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14392, 3393, 2011
R_{int}	0.120
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.604
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.079, 0.230, 1.02
No. of reflections	3393
No. of parameters	274
No. of restraints	15
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	1.68, −0.61

Computer programs: *COSMO* (Bruker, 2009), *SAINT* (Bruker, 2014), *SHELXT2018/2* (Sheldrick, 2015), *SHELXL2018/3* (Sheldrick, 2015), *CrystalMaker X* (Palmer, 2020), and *OLEX2* (Dolomanov *et al.*, 2009).

3-ylamino)ethyl)nicotinamide (pen) (100 mg, 0.37 mmol) and 0.75 ml of a 1.0 *M* NaOH solution were placed into 10 ml distilled H$_2$O in a Teflon-lined acid digestion bomb. The bomb was sealed and heated in an oven at 373 K for 48 h, and then cooled slowly to 273 K. Green crystals of the title complex were obtained in 43% yield.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The O3W position disordered across an inversion center was treated with a PART −1 command. Water H atom positions are refined, but suitably restrained with 0.84 (2) Å target values for O—H bonds, 1.36 (2) Å target values for H$\cdots$H distances, and suitable *DFIX* commands for hydrogen-bonding H$\cdots$O distances (with EQIV commands added as needed). The amine H-atom position was allowed to refine with an N—H distance restraint of 0.88 (2) Å.

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full crystallographic data

Poly[[bis[μ_4-3-(2-carboxylatophenyl)propionato]{*N*-[2-(pyridine-3-amido)ethyl]-nicotinamide}dicopper(II)] pentahydrate]

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Poly[[bis[μ_4-3-(2-carboxylatophenyl)propionato]{*N*-[2-(pyridine-3-amido)ethyl]nicotinamide}dicopper(II)] pentahydrate]

Crystal data

[Cu$_2$(C$_{10}$H$_8$O$_4$)$_2$(C$_{14}$H$_{14}$N$_4$O$_2$)]·5H$_2$O	$F(000) = 1800$
$M_r = 871.78$	$D_x = 1.561$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 27.558$ (10) Å	Cell parameters from 2345 reflections
$b = 14.873$ (5) Å	$\theta = 2.6$–24.4°
$c = 9.146$ (3) Å	$\mu = 1.22$ mm^{-1}
$\beta = 98.396$ (4)°	$T = 173$ K
$V = 3709$ (2) Å^3	Block, green
$Z = 4$	0.28 × 0.16 × 0.11 mm

Data collection

Bruker APEXII CCD diffractometer	3393 independent reflections
φ and ω scans	2011 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)	$R_{int} = 0.120$
	$\theta_{max} = 25.4°$, $\theta_{min} = 1.5°$
$T_{min} = 0.560$, $T_{max} = 0.745$	$h = -33 \rightarrow 33$
14392 measured reflections	$k = -17 \rightarrow 17$
	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	Hydrogen site location: mixed
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.079$	
$wR(F^2) = 0.230$	$w = 1/[\sigma^2(F_o^2) + (0.1316P)^2]$
$S = 1.02$	where $P = (F_o^2 + 2F_c^2)/3$
3393 reflections	$(\Delta/\sigma)_{max} < 0.001$
274 parameters	$\Delta\rho_{max} = 1.68$ e Å^{-3}
15 restraints	$\Delta\rho_{min} = -0.61$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cu1	0.28340 (3)	0.31333 (5)	0.51554 (10)	0.0264 (3)	
O1	0.4310 (2)	0.6336 (4)	0.8536 (6)	0.0531 (16)	
O2	0.2511 (2)	0.3449 (3)	0.3163 (6)	0.0394 (14)	
O3	0.19296 (19)	0.2383 (3)	0.2891 (5)	0.0327 (13)	
O4	0.23078 (19)	0.6236 (3)	0.1031 (6)	0.0369 (13)	
O5	0.17254 (18)	0.7279 (3)	0.0656 (6)	0.0352 (13)	
N1	0.3245 (2)	0.4382 (4)	0.5434 (7)	0.0282 (14)	
N2	0.4359 (3)	0.4863 (5)	0.9037 (8)	0.0406 (17)	
H2	0.435 (3)	0.432 (3)	0.868 (9)	0.049*	
C1	0.4759 (3)	0.4959 (6)	1.0262 (9)	0.044 (2)	
H1A	0.476383	0.442866	1.091850	0.053*	
H1B	0.470134	0.549866	1.084528	0.053*	
C2	0.4170 (3)	0.5543 (5)	0.8263 (9)	0.037 (2)	
C3	0.3778 (3)	0.5378 (5)	0.7005 (8)	0.0319 (18)	
C4	0.3592 (3)	0.4538 (5)	0.6571 (8)	0.0281 (17)	
H4	0.372276	0.403411	0.713309	0.034*	
C5	0.3067 (2)	0.5096 (4)	0.4656 (7)	0.0219 (15)	
H5	0.281838	0.499813	0.383485	0.026*	
C6	0.3218 (3)	0.5968 (5)	0.4963 (9)	0.0368 (19)	
H6	0.308207	0.645667	0.437001	0.044*	
C7	0.3571 (3)	0.6102 (5)	0.6154 (9)	0.039 (2)	
H7	0.367833	0.669622	0.640970	0.047*	
C8	0.2140 (3)	0.3066 (5)	0.2454 (8)	0.0268 (16)	
C9	0.1944 (3)	0.3433 (4)	0.0944 (8)	0.0283 (17)	
H9A	0.160390	0.321624	0.065279	0.034*	
H9B	0.214539	0.320015	0.021644	0.034*	
C10	0.1947 (3)	0.4467 (4)	0.0900 (8)	0.0278 (17)	
H10A	0.227492	0.467709	0.135551	0.033*	
H10B	0.190022	0.465789	−0.014842	0.033*	
C11	0.1564 (3)	0.4942 (5)	0.1665 (7)	0.0254 (16)	
C12	0.1229 (3)	0.4454 (5)	0.2329 (8)	0.0333 (18)	
H12	0.125034	0.381659	0.232085	0.040*	
C13	0.0869 (3)	0.4842 (6)	0.2995 (10)	0.045 (2)	
H13	0.065171	0.448100	0.346293	0.054*	
C14	0.0824 (3)	0.5796 (6)	0.2977 (10)	0.045 (2)	
H14	0.056980	0.608167	0.340443	0.054*	
C15	0.1155 (3)	0.6296 (5)	0.2330 (8)	0.0349 (19)	
H15	0.112726	0.693235	0.230924	0.042*	
C16	0.1529 (3)	0.5884 (5)	0.1704 (8)	0.0299 (17)	
C17	0.1880 (3)	0.6497 (5)	0.1074 (8)	0.0286 (17)	
O1W	0.4372 (5)	0.2956 (5)	0.8813 (11)	0.120 (4)	
H1WA	0.449 (6)	0.275 (9)	0.807 (10)	0.181*	
H1WB	0.445 (5)	0.259 (4)	0.951 (7)	0.181*	
O2W	0.4262 (3)	0.2494 (5)	0.5930 (8)	0.088 (3)	
H2WA	0.3977 (19)	0.232 (7)	0.557 (11)	0.133*	

H2WB	0.438 (2)	0.273 (6)	0.522 (9)	0.133*	
O3W	0.4849 (7)	0.2581 (12)	1.166 (2)	0.111 (6)	0.5
H3WA	0.464 (4)	0.281 (12)	1.21 (2)	0.167*	0.5
H3WB	0.501 (2)	0.300 (9)	1.134 (16)	0.167*	0.5

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0419 (6)	0.0104 (5)	0.0247 (5)	−0.0009 (4)	−0.0023 (4)	0.0007 (4)
O1	0.063 (4)	0.049 (4)	0.043 (4)	−0.012 (3)	−0.006 (3)	−0.012 (3)
O2	0.052 (4)	0.026 (3)	0.036 (3)	−0.011 (3)	−0.011 (3)	0.006 (2)
O3	0.047 (3)	0.020 (3)	0.026 (3)	−0.005 (2)	−0.010 (2)	0.003 (2)
O4	0.040 (3)	0.017 (3)	0.055 (4)	−0.003 (2)	0.011 (3)	0.004 (2)
O5	0.042 (3)	0.022 (3)	0.041 (3)	0.001 (2)	0.005 (3)	0.008 (2)
N1	0.045 (4)	0.010 (3)	0.029 (3)	−0.001 (3)	0.005 (3)	0.001 (3)
N2	0.046 (4)	0.036 (4)	0.038 (4)	−0.004 (3)	0.000 (3)	0.003 (3)
C1	0.043 (5)	0.048 (6)	0.039 (5)	−0.004 (4)	0.000 (4)	0.001 (4)
C2	0.046 (5)	0.034 (5)	0.031 (5)	−0.013 (4)	0.009 (4)	0.001 (4)
C3	0.039 (5)	0.026 (4)	0.029 (4)	−0.011 (3)	−0.001 (3)	0.000 (3)
C4	0.037 (4)	0.024 (4)	0.021 (4)	0.002 (3)	−0.004 (3)	0.007 (3)
C5	0.025 (4)	0.022 (4)	0.020 (4)	−0.001 (3)	0.006 (3)	0.000 (3)
C6	0.049 (5)	0.019 (4)	0.043 (5)	0.000 (3)	0.009 (4)	0.006 (4)
C7	0.054 (5)	0.020 (4)	0.043 (5)	−0.009 (4)	0.006 (4)	−0.007 (4)
C8	0.041 (4)	0.015 (4)	0.024 (4)	0.001 (3)	0.000 (3)	0.001 (3)
C9	0.053 (5)	0.011 (3)	0.019 (4)	−0.001 (3)	−0.003 (3)	−0.004 (3)
C10	0.048 (5)	0.012 (4)	0.022 (4)	−0.002 (3)	0.001 (3)	0.000 (3)
C11	0.036 (4)	0.018 (4)	0.020 (4)	−0.003 (3)	−0.004 (3)	0.004 (3)
C12	0.046 (5)	0.024 (4)	0.029 (4)	−0.002 (3)	0.002 (4)	0.006 (3)
C13	0.051 (5)	0.035 (5)	0.048 (6)	−0.007 (4)	0.007 (4)	0.010 (4)
C14	0.039 (5)	0.050 (6)	0.048 (5)	0.004 (4)	0.011 (4)	0.001 (4)
C15	0.047 (5)	0.028 (4)	0.029 (4)	0.002 (4)	0.003 (4)	−0.005 (3)
C16	0.037 (4)	0.024 (4)	0.026 (4)	−0.002 (3)	−0.002 (3)	0.009 (3)
C17	0.041 (5)	0.013 (4)	0.028 (4)	−0.004 (3)	−0.004 (3)	−0.002 (3)
O1W	0.219 (12)	0.049 (5)	0.081 (7)	0.003 (6)	−0.018 (8)	−0.001 (5)
O2W	0.125 (7)	0.055 (5)	0.079 (6)	−0.016 (5)	−0.009 (5)	0.009 (4)
O3W	0.129 (17)	0.087 (13)	0.116 (16)	−0.012 (12)	0.015 (13)	0.014 (11)

Geometric parameters (Å, º)

Cu1—Cu1[i]	2.6201 (18)	C6—C7	1.365 (11)
Cu1—O2	1.965 (5)	C7—H7	0.9500
Cu1—O3[i]	1.967 (5)	C8—C9	1.510 (9)
Cu1—O4[ii]	1.991 (5)	C9—H9A	0.9900
Cu1—O5[iii]	1.975 (5)	C9—H9B	0.9900
Cu1—N1	2.172 (6)	C9—C10	1.538 (9)
O1—C2	1.255 (9)	C10—H10A	0.9900
O2—C8	1.263 (9)	C10—H10B	0.9900
O3—C8	1.263 (8)	C10—C11	1.522 (10)

O4—C17	1.247 (8)	C11—C12	1.383 (10)
O5—C17	1.278 (8)	C11—C16	1.405 (10)
N1—C4	1.325 (9)	C12—H12	0.9500
N1—C5	1.332 (8)	C12—C13	1.366 (11)
N2—H2	0.87 (2)	C13—H13	0.9500
N2—C1	1.460 (10)	C13—C14	1.424 (12)
N2—C2	1.299 (10)	C14—H14	0.9500
C1—C1^{iv}	1.480 (16)	C14—C15	1.376 (11)
C1—H1A	0.9900	C15—H15	0.9500
C1—H1B	0.9900	C15—C16	1.393 (10)
C2—C3	1.479 (11)	C16—C17	1.505 (10)
C3—C4	1.387 (10)	O1W—H1WA	0.85 (2)
C3—C7	1.400 (11)	O1W—H1WB	0.85 (2)
C4—H4	0.9500	O2W—H2WA	0.846 (18)
C5—H5	0.9500	O2W—H2WB	0.85 (2)
C5—C6	1.379 (10)	O3W—H3WA	0.84 (2)
C6—H6	0.9500	O3W—H3WB	0.84 (2)
O2—Cu1—Cu1^{i}	81.66 (15)	C7—C6—C5	117.3 (7)
O2—Cu1—O3^{i}	168.9 (2)	C7—C6—H6	121.3
O2—Cu1—O4^{ii}	90.1 (2)	C3—C7—H7	119.5
O2—Cu1—O5^{iii}	91.5 (2)	C6—C7—C3	121.1 (7)
O2—Cu1—N1	93.6 (2)	C6—C7—H7	119.5
O3^{i}—Cu1—Cu1^{i}	87.24 (15)	O2—C8—O3	125.1 (7)
O3^{i}—Cu1—O4^{ii}	89.0 (2)	O2—C8—C9	117.5 (6)
O3^{i}—Cu1—O5^{iii}	87.1 (2)	O3—C8—C9	117.4 (6)
O3^{i}—Cu1—N1	97.5 (2)	C8—C9—H9A	109.1
O4^{ii}—Cu1—Cu1^{i}	80.87 (16)	C8—C9—H9B	109.1
O4^{ii}—Cu1—N1	87.0 (2)	C8—C9—C10	112.6 (6)
O5^{iii}—Cu1—Cu1^{i}	87.57 (15)	H9A—C9—H9B	107.8
O5^{iii}—Cu1—O4^{ii}	168.0 (2)	C10—C9—H9A	109.1
O5^{iii}—Cu1—N1	104.8 (2)	C10—C9—H9B	109.1
N1—Cu1—Cu1^{i}	166.94 (17)	C9—C10—H10A	108.2
C8—O2—Cu1	126.3 (5)	C9—C10—H10B	108.2
C8—O3—Cu1^{i}	119.7 (5)	H10A—C10—H10B	107.3
C17—O4—Cu1^{v}	127.8 (5)	C11—C10—C9	116.5 (6)
C17—O5—Cu1^{vi}	120.0 (5)	C11—C10—H10A	108.2
C4—N1—Cu1	123.1 (5)	C11—C10—H10B	108.2
C4—N1—C5	116.6 (6)	C12—C11—C10	120.6 (6)
C5—N1—Cu1	118.2 (5)	C12—C11—C16	117.4 (7)
C1—N2—H2	111 (6)	C16—C11—C10	121.9 (6)
C2—N2—H2	122 (6)	C11—C12—H12	118.3
C2—N2—C1	122.7 (7)	C13—C12—C11	123.3 (7)
N2—C1—C1^{iv}	111.9 (9)	C13—C12—H12	118.3
N2—C1—H1A	109.2	C12—C13—H13	120.6
N2—C1—H1B	109.2	C12—C13—C14	118.9 (8)
C1^{iv}—C1—H1A	109.2	C14—C13—H13	120.6
C1^{iv}—C1—H1B	109.2	C13—C14—H14	120.6

H1A—C1—H1B	107.9	C15—C14—C13	118.8 (8)
O1—C2—N2	122.4 (8)	C15—C14—H14	120.6
O1—C2—C3	118.7 (7)	C14—C15—H15	119.4
N2—C2—C3	119.0 (7)	C14—C15—C16	121.1 (8)
C4—C3—C2	124.7 (7)	C16—C15—H15	119.4
C4—C3—C7	115.5 (7)	C11—C16—C17	123.0 (7)
C7—C3—C2	119.8 (7)	C15—C16—C11	120.4 (7)
N1—C4—C3	125.2 (7)	C15—C16—C17	116.6 (7)
N1—C4—H4	117.4	O4—C17—O5	123.4 (7)
C3—C4—H4	117.4	O4—C17—C16	119.1 (6)
N1—C5—H5	117.9	O5—C17—C16	117.4 (7)
N1—C5—C6	124.3 (7)	H1WA—O1W—H1WB	107 (3)
C6—C5—H5	117.9	H2WA—O2W—H2WB	106 (3)
C5—C6—H6	121.3	H3WA—O3W—H3WB	108 (4)
Cu1—O2—C8—O3	−3.5 (11)	C4—C3—C7—C6	−1.4 (12)
Cu1—O2—C8—C9	178.6 (5)	C5—N1—C4—C3	0.2 (11)
Cu1^i—O3—C8—O2	2.1 (10)	C5—C6—C7—C3	1.4 (12)
Cu1^i—O3—C8—C9	179.9 (5)	C7—C3—C4—N1	0.6 (11)
Cu1^v—O4—C17—O5	−6.6 (11)	C8—C9—C10—C11	−72.9 (8)
Cu1^v—O4—C17—C16	175.9 (5)	C9—C10—C11—C12	−1.4 (10)
Cu1^{vi}—O5—C17—O4	1.6 (10)	C9—C10—C11—C16	179.9 (6)
Cu1^{vi}—O5—C17—C16	179.1 (5)	C10—C11—C12—C13	−178.1 (7)
Cu1—N1—C4—C3	−163.0 (6)	C10—C11—C16—C15	175.8 (7)
Cu1—N1—C5—C6	163.9 (6)	C10—C11—C16—C17	−3.5 (11)
O1—C2—C3—C4	179.3 (8)	C11—C12—C13—C14	1.8 (13)
O1—C2—C3—C7	−0.3 (12)	C11—C16—C17—O4	−28.2 (11)
O2—C8—C9—C10	−40.7 (10)	C11—C16—C17—O5	154.2 (7)
O3—C8—C9—C10	141.3 (7)	C12—C11—C16—C15	−3.0 (11)
N1—C5—C6—C7	−0.7 (11)	C12—C11—C16—C17	177.7 (7)
N2—C2—C3—C4	−0.1 (12)	C12—C13—C14—C15	−2.0 (13)
N2—C2—C3—C7	−179.7 (7)	C13—C14—C15—C16	−0.2 (12)
C1—N2—C2—O1	−1.8 (13)	C14—C15—C16—C11	2.7 (12)
C1—N2—C2—C3	177.7 (7)	C14—C15—C16—C17	−177.9 (7)
C2—N2—C1—C1^{iv}	−80.0 (12)	C15—C16—C17—O4	152.4 (7)
C2—C3—C4—N1	−179.0 (7)	C15—C16—C17—O5	−25.2 (10)
C2—C3—C7—C6	178.3 (7)	C16—C11—C12—C13	0.7 (11)
C4—N1—C5—C6	−0.1 (10)		

Symmetry codes: (i) −x+1/2, −y+1/2, −z+1; (ii) x, −y+1, z+1/2; (iii) −x+1/2, y−1/2, −z+1/2; (iv) −x+1, −y+1, −z+2; (v) x, −y+1, z−1/2; (vi) −x+1/2, y+1/2, −z+1/2.

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O1W	0.87 (2)	2.03 (4)	2.844 (10)	155 (8)
C5—H5···O2	0.95	2.50	3.099 (9)	121
C6—H6···O3^{vi}	0.95	2.48	3.332 (9)	149
O1W—H1WA···O2W	0.85 (2)	2.00 (11)	2.698 (13)	139 (15)

O1*W*—H1*WB*···O3*W*	0.85 (2)	2.10 (2)	2.79 (2)	139 (5)
O2*W*—H2*WA*···O5^{iii}	0.85 (2)	2.09 (2)	2.909 (10)	162 (7)
O2*W*—H2*WB*···O1^{v}	0.85 (2)	2.06 (2)	2.816 (9)	147 (5)
O3*W*—H3*WA*···O1^{ii}	0.84 (2)	2.10 (2)	2.917 (19)	162 (9)
O3*W*—H3*WB*···O1^{iv}	0.84 (2)	2.10 (2)	2.848 (19)	147 (6)

Symmetry codes: (ii) x, $-y+1$, $z+1/2$; (iii) $-x+1/2$, $y-1/2$, $-z+1/2$; (iv) $-x+1$, $-y+1$, $-z+2$; (v) x, $-y+1$, $z-1/2$; (vi) $-x+1/2$, $y+1/2$, $-z+1/2$.