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catena-Poly[[[aquabis(acetato-κO)-copper(II)]-μ-1,3-di-4-pyridylpropane-κ^2N:N'] monohydrate]

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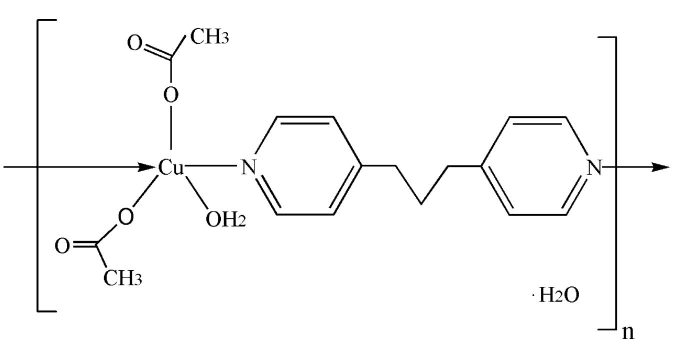
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.009 Å; R factor = 0.047; wR factor = 0.117; data-to-parameter ratio = 15.1.

In the title complex, $\{[Cu(CH_3COO)_2(C_{13}H_{14}N_2)(H_2O)]\cdot H_2O\}_n$, the Cu atom is five-coordinated in a distorted square-pyramidal geometry by one O atom of the coordinated water molecule, two O atoms from two acetate anions and two N atoms from two 1,3-di-4-pyridylpropane (dpp) ligands. The dpp ligands bridge the Cu atoms to form a zigzag chain. The crystal structure involves O—H···O hydrogen bonds.

Related literature

For related literature, see: Carlucci *et al.* (2002); Dai *et al.* (2004); Hou *et al.* (2003); Konar *et al.* (2004); Lee *et al.* (2004); Li *et al.* (2004, 2005); Madalan *et al.* (2005); Manna *et al.* (2005); Nassimbeni *et al.* (2004); Niu *et al.* (2003); Rarig & Zubieta (2003); Sunahara *et al.* (2004); Tong *et al.* (2002); Xia *et al.* (2004).



Experimental

Crystal data

$[Cu(C_2H_3O_2)_2(C_{13}H_{14}N_2)(H_2O)]\cdot H_2O$
M_r = 415.92
Orthorhombic, $Fdd2$
a = 18.988 (3) Å
b = 32.249 (6) Å
c = 12.883 (2) Å
V = 7889 (2) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 1.14 mm^{-1}
T = 291 (2) K
0.26 × 0.18 × 0.10 mm

Data collection

Bruker APEX II CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.757, T_{max} = 0.895
11662 measured reflections
3599 independent reflections
2517 reflections with $I > 2\sigma(I)$
R_{int} = 0.062

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.118
S = 1.03
3599 reflections
238 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}
Absolute structure: Flack (1983), 1675 Friedel pairs
Flack parameter: −0.03 (2)

Table 1
Selected geometric parameters (Å, °).

Cu1—O3	1.952 (4)	Cu1—N2^i	2.037 (4)
Cu1—O1	1.960 (4)	Cu1—O5	2.371 (5)
Cu1—N1	2.011 (4)		
O3—Cu1—O1	172.88 (18)	O1—Cu1—O5	96.93 (19)
O1—Cu1—N1	91.35 (17)	N1—Cu1—O5	89.59 (17)
O1—Cu1—N2^i	89.17 (17)	N2^i—Cu1—O5	98.15 (18)
O3—Cu1—O5	90.03 (17)		

Symmetry code: (i) $-x+\frac{7}{4}, y-\frac{1}{4}, z-\frac{3}{4}$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H1W···O2	0.83	1.96	2.663 (8)	142
O5—H2W···O6^{ii}	0.83	1.99	2.795 (8)	164
O6—H3W···O4	0.83	1.96	2.730 (7)	154
O6—H4W···O1^{iii}	0.85	2.07	2.916 (7)	180

Symmetry codes: (ii) $-x+\frac{7}{4}, y+\frac{1}{4}, z-\frac{1}{4}$; (iii) $x-\frac{1}{4}, -y+\frac{1}{4}, z-\frac{1}{4}$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2004); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2117).

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supplementary materials

Acta Cryst. (2007). E**63**, m2133-m2134 [**doi:10.1107/S160053680703334X**]

catena-Poly[[[aquabis(acetato-*κO*)copper(II)]-*μ*-1,3-di-4-pyridylpropane-$\kappa^2 N$:N'] monohydrate]

Z.-X. Du and J.-X. Li

Comment

The ligand 1,3-di-4-pyridylpropane (dpp) has been extensively studied in recent years due to its strong coordination capability and bridging function. Here we report the structure of a new coordination polymer (I) (Fig. 1). The polymeric chain is assembled of $[Cu(C_{13}H_{14}N_2)(CH_3COO)_2(H_2O)]\cdot H_2O$ with the five coordinated Cu^{II}. The coordination sphere includes the coordinated water molecule, two carboxyl O atoms from two acetate anions and two pyridyl N from two 1,3-di-4-pyridylpropane(dpp) ligands (Table 1). The plane N1/O3/N2A/O1 defines the base of the pyramid while water O5 is the apex. The distance from Cu to the least-squares plane N1/O3/N2A/O1 is 0.1272 (3) Å. The dpp ligand acts as a bridging ligand linking neighbouring Cu^{II} atoms into a zigzag chain with the Cu1···Cu1 ($-x + 7/4$, $y - 1/4$, $z - 3/4$) separation distance of 12.851 (2) Å.

In the crystal structure of (I), there is π-π stacking interactions between the adjacent pyridine rings of neighbouring chains. The dihedral angle of aromatics involved in stacking is 8.788 (1) °. Interplanar average distance and ring-centroid separation distance are 3.441 (1) Å and 3.701 (4) Å, respectively. The chain structure is crosswise arranged into two-dimensional network (Fig. 2) by π-π stacking. The coordinated and uncoordinate water molecules, and carboxyl group take part in intermolecular hydrogen bonding (Table 2) stabilizing the structure.

Experimental

The ligand dpp (1 mmol, 0.2 g) was dissolved in a mixture water - methanol (*v*/*v* 1:1, 20 ml). To this solution, $Cu(CH_3COO)_2$. $4H_2O$ (1 mmol, 0.26 g) was added and the resulting mixture was stirred and refluxed at 353 K for 3 h. Then the reaction mixture was cooled to room temperature. After filtration and evaporation in air for five days, dark-blue block-shaped crystals were obtained in the yield of 45%.

Refinement

H atoms bonded to C atoms were positioned geometrically with C—H distance 0.93–0.97 Å, and treated as riding atoms with U_{iso}(H)=1.2U_{eq}(C). H atoms bonded to O atoms were located in a difference Fourier map and refined isotropically.

Figures

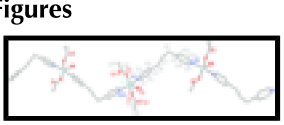

Fig. 1. A segment of the polymeric structure of (I) with the atom numbering scheme. H atoms and solvent molecules have been omitted for clarity. Labelling A corresponds to symmetry operation $-x + 7/4$, $y - 1/4$, $z - 3/4$.

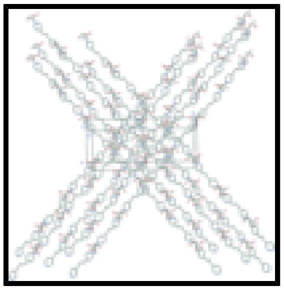

Fig. 2. Packing of (I) showing the intercrossed chains in the *bc* plane stabilized by π-π stacking and hydrogen bonds. H atoms bonded to C have been omitted for clarity.

catena-Poly[[[aquabis(acetato-κ*O*)copper(II)]-μ-1,3-di-4-pyridylpropane-\ κ^2*N*:*N*'] monohydrate]

Crystal data

$[Cu(C_2H_3O_2)_2(C_{13}H_{14}N_2)(H_2O)]\cdot H_2O$	F_{000} = 3472
M_r = 415.92	D_x = 1.401 Mg m^{-3}
Orthorhombic, *Fdd*2	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: F 2 2d	Cell parameters from 1579 reflections
a = 18.988 (3) Å	θ = 2.5–17.4°
b = 32.249 (6) Å	μ = 1.14 mm^{-1}
c = 12.883 (2) Å	*T* = 291 (2) K
V = 7889 (2) Å^3	Block, blue
Z = 16	0.26 × 0.18 × 0.10 mm

Data collection

Bruker APEX II CCD area-detector diffractometer	3599 independent reflections
Radiation source: fine-focus sealed tube	2517 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.062
T = 291(2) K	θ_{max} = 25.5°
φ and ω scans	θ_{min} = 2.5°
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -22 \rightarrow 21$
T_{min} = 0.757, T_{max} = 0.895	$k = -38 \rightarrow 38$
11662 measured reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.047	$w = 1/[\sigma^2(F_o^2) + (0.0455P)^2 + 4.4493P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.118	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.03	$\Delta\rho_{max}$ = 0.37 e Å^{-3}
3599 reflections	$\Delta\rho_{min}$ = −0.34 e Å^{-3}

238 parameters	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
1 restraint	Extinction coefficient: 0.00018 (5)
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 1675 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: −0.03 (2)

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.94362 (3)	0.221410 (19)	0.13402 (4)	0.0506 (2)
O1	1.0258 (2)	0.21314 (13)	0.2238 (3)	0.0634 (11)
O2	1.0911 (3)	0.26709 (19)	0.1777 (4)	0.0951 (17)
O3	0.8590 (2)	0.22242 (12)	0.0479 (3)	0.0566 (10)
O4	0.8358 (2)	0.16359 (14)	0.1289 (5)	0.0794 (12)
N1	0.8914 (2)	0.25056 (13)	0.2485 (3)	0.0468 (11)
N2	0.7602 (2)	0.43467 (13)	0.7749 (3)	0.0487 (11)
C1	0.8983 (3)	0.24184 (17)	0.3503 (4)	0.0498 (14)
H1	0.9299	0.2213	0.3697	0.060*
C2	0.8608 (3)	0.26183 (17)	0.4273 (4)	0.0499 (14)
H2	0.8683	0.2549	0.4965	0.060*
C3	0.8124 (3)	0.29185 (14)	0.4024 (4)	0.0434 (13)
C4	0.8042 (3)	0.30058 (19)	0.2972 (5)	0.0552 (15)
H4	0.7718	0.3205	0.2758	0.066*

C5	0.8443 (3)	0.27966 (17)	0.2248 (4)	0.0551 (15)
H5A	0.8380	0.2863	0.1552	0.066*
C6	0.7696 (3)	0.31317 (18)	0.4853 (4)	0.0553 (15)
H6A	0.7473	0.2919	0.5272	0.066*
H6B	0.8020	0.3281	0.5302	0.066*
C7	0.7137 (3)	0.34300 (18)	0.4510 (5)	0.0579 (16)
H7A	0.6850	0.3299	0.3980	0.069*
H7B	0.7360	0.3671	0.4201	0.069*
C8	0.6663 (3)	0.35713 (19)	0.5390 (5)	0.0657 (17)
H8A	0.6275	0.3729	0.5096	0.079*
H8B	0.6464	0.3328	0.5721	0.079*
C9	0.7015 (3)	0.38344 (15)	0.6215 (5)	0.0503 (14)
C10	0.7441 (3)	0.41616 (17)	0.5972 (4)	0.0529 (15)
H10	0.7545	0.4217	0.5281	0.064*
C11	0.7718 (3)	0.44097 (17)	0.6741 (4)	0.0517 (15)
H11	0.8000	0.4632	0.6547	0.062*
C12	0.7200 (4)	0.40184 (17)	0.7989 (5)	0.0627 (16)
H12	0.7115	0.3965	0.8687	0.075*
C13	0.6905 (3)	0.37572 (18)	0.7271 (5)	0.0607 (16)
H13	0.6636	0.3532	0.7483	0.073*
C14	1.0826 (4)	0.2345 (3)	0.2237 (5)	0.0641 (17)
C15	1.1433 (4)	0.2170 (3)	0.2868 (7)	0.101 (3)
H15A	1.1846	0.2336	0.2759	0.152*
H15B	1.1525	0.1890	0.2652	0.152*
H15C	1.1311	0.2172	0.3591	0.152*
C16	0.8226 (3)	0.1898 (2)	0.0627 (5)	0.0638 (17)
C17	0.7590 (4)	0.1858 (3)	−0.0080 (6)	0.094 (2)
H17A	0.7302	0.1631	0.0149	0.141*
H17B	0.7745	0.1807	−0.0778	0.141*
H17C	0.7322	0.2110	−0.0059	0.141*
O5	0.9779 (3)	0.28664 (15)	0.0658 (4)	0.0954 (16)
H1W	1.0175	0.2760	0.0731	0.143*
H2W	0.9795	0.3068	0.0257	0.143*
O6	0.7594 (3)	0.09240 (19)	0.1507 (5)	0.133 (2)
H3W	0.7813	0.1140	0.1647	0.200*
H4W	0.7643	0.0762	0.0993	0.200*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0534 (4)	0.0558 (4)	0.0425 (3)	0.0047 (3)	−0.0012 (4)	−0.0031 (3)
O1	0.063 (3)	0.074 (3)	0.052 (3)	0.013 (2)	−0.007 (2)	0.002 (2)
O2	0.088 (4)	0.113 (4)	0.084 (4)	−0.015 (3)	−0.006 (3)	0.018 (3)
O3	0.056 (3)	0.062 (3)	0.052 (2)	0.006 (2)	−0.007 (2)	−0.0083 (19)
O4	0.077 (3)	0.077 (3)	0.085 (3)	−0.011 (2)	−0.008 (3)	0.002 (3)
N1	0.049 (3)	0.046 (3)	0.045 (3)	0.003 (2)	0.000 (2)	0.001 (2)
N2	0.057 (3)	0.047 (3)	0.042 (3)	−0.004 (2)	0.003 (2)	0.004 (2)
C1	0.047 (3)	0.052 (3)	0.051 (4)	0.004 (3)	−0.003 (3)	0.005 (3)

C2	0.051 (4)	0.053 (3)	0.046 (3)	−0.001 (3)	−0.004 (3)	0.002 (3)
C3	0.044 (3)	0.037 (2)	0.049 (4)	−0.007 (2)	−0.005 (3)	−0.008 (2)
C4	0.067 (4)	0.052 (3)	0.046 (3)	0.013 (3)	−0.009 (3)	−0.003 (3)
C5	0.070 (4)	0.056 (3)	0.039 (3)	0.014 (3)	−0.006 (3)	0.000 (3)
C6	0.055 (4)	0.057 (3)	0.054 (4)	−0.007 (3)	−0.002 (3)	−0.013 (3)
C7	0.062 (4)	0.053 (3)	0.059 (4)	0.010 (3)	−0.008 (3)	−0.018 (3)
C8	0.053 (4)	0.069 (4)	0.075 (4)	0.007 (3)	−0.002 (3)	−0.023 (3)
C9	0.044 (3)	0.041 (3)	0.066 (4)	0.003 (2)	−0.002 (3)	−0.012 (3)
C10	0.056 (4)	0.057 (3)	0.046 (3)	0.004 (3)	0.002 (3)	−0.009 (3)
C11	0.054 (4)	0.050 (3)	0.051 (4)	−0.005 (3)	−0.002 (3)	0.000 (3)
C12	0.086 (5)	0.052 (3)	0.050 (3)	−0.007 (3)	0.000 (3)	0.007 (3)
C13	0.070 (4)	0.049 (3)	0.064 (4)	−0.016 (3)	0.000 (3)	0.003 (3)
C14	0.048 (4)	0.099 (5)	0.046 (4)	0.004 (4)	0.007 (3)	−0.014 (4)
C15	0.058 (5)	0.150 (8)	0.095 (6)	0.016 (5)	−0.026 (5)	−0.007 (5)
C16	0.055 (4)	0.079 (5)	0.057 (4)	0.009 (4)	0.001 (3)	−0.026 (4)
C17	0.063 (5)	0.135 (7)	0.084 (5)	0.003 (5)	−0.013 (4)	−0.050 (5)
O5	0.079 (3)	0.094 (4)	0.113 (4)	−0.001 (3)	0.011 (3)	0.027 (3)
O6	0.169 (6)	0.124 (5)	0.107 (5)	−0.062 (4)	0.025 (5)	−0.015 (4)

Geometric parameters (Å, °)

Cu1—O3	1.952 (4)	C7—C8	1.517 (8)
Cu1—O1	1.960 (4)	C7—H7A	0.9700
Cu1—N1	2.011 (4)	C7—H7B	0.9700
Cu1—N2^{i}	2.037 (4)	C8—C9	1.516 (8)
Cu1—O5	2.371 (5)	C8—H8A	0.9700
O1—C14	1.280 (8)	C8—H8B	0.9700
O2—C14	1.217 (8)	C9—C10	1.366 (7)
O3—C16	1.275 (8)	C9—C13	1.398 (8)
O4—C16	1.226 (8)	C10—C11	1.377 (7)
N1—C5	1.332 (6)	C10—H10	0.9300
N1—C1	1.347 (6)	C11—H11	0.9300
N2—C11	1.332 (6)	C12—C13	1.370 (8)
N2—C12	1.342 (7)	C12—H12	0.9300
N2—Cu1^{ii}	2.037 (4)	C13—H13	0.9300
C1—C2	1.381 (7)	C14—C15	1.520 (9)
C1—H1	0.9300	C15—H15A	0.9600
C2—C3	1.373 (7)	C15—H15B	0.9600
C2—H2	0.9300	C15—H15C	0.9600
C3—C4	1.393 (8)	C16—C17	1.517 (9)
C3—C6	1.508 (7)	C17—H17A	0.9600
C4—C5	1.380 (8)	C17—H17B	0.9600
C4—H4	0.9300	C17—H17C	0.9600
C5—H5A	0.9300	O5—H1W	0.8307
C6—C7	1.500 (8)	O5—H2W	0.8299
C6—H6A	0.9700	O6—H3W	0.8316
C6—H6B	0.9700	O6—H4W	0.8492
O3—Cu1—O1	172.88 (18)	H7A—C7—H7B	107.8

O3—Cu1—N1	90.19 (17)	C9—C8—C7	115.5 (5)
O1—Cu1—N1	91.35 (17)	C9—C8—H8A	108.4
O3—Cu1—N2^{i}	88.36 (17)	C7—C8—H8A	108.4
O1—Cu1—N2^{i}	89.17 (17)	C9—C8—H8B	108.4
N1—Cu1—N2^{i}	172.12 (18)	C7—C8—H8B	108.4
O3—Cu1—O5	90.03 (17)	H8A—C8—H8B	107.5
O1—Cu1—O5	96.93 (19)	C10—C9—C13	116.7 (5)
N1—Cu1—O5	89.59 (17)	C10—C9—C8	122.2 (6)
N2^{i}—Cu1—O5	98.15 (18)	C13—C9—C8	121.1 (5)
C14—O1—Cu1	126.6 (4)	C9—C10—C11	120.7 (5)
C16—O3—Cu1	110.4 (4)	C9—C10—H10	119.7
C5—N1—C1	115.8 (5)	C11—C10—H10	119.7
C5—N1—Cu1	119.5 (4)	N2—C11—C10	123.3 (5)
C1—N1—Cu1	124.6 (4)	N2—C11—H11	118.4
C11—N2—C12	116.1 (5)	C10—C11—H11	118.4
C11—N2—Cu1^{ii}	120.8 (4)	N2—C12—C13	124.2 (6)
C12—N2—Cu1^{ii}	123.0 (4)	N2—C12—H12	117.9
N1—C1—C2	123.5 (5)	C13—C12—H12	117.9
N1—C1—H1	118.3	C12—C13—C9	119.1 (5)
C2—C1—H1	118.3	C12—C13—H13	120.5
C3—C2—C1	120.4 (5)	C9—C13—H13	120.5
C3—C2—H2	119.8	O2—C14—O1	125.3 (7)
C1—C2—H2	119.8	O2—C14—C15	118.8 (7)
C2—C3—C4	116.4 (5)	O1—C14—C15	115.9 (7)
C2—C3—C6	121.1 (5)	C14—C15—H15A	109.5
C4—C3—C6	122.5 (5)	C14—C15—H15B	109.5
C5—C4—C3	119.8 (5)	H15A—C15—H15B	109.5
C5—C4—H4	120.1	C14—C15—H15C	109.5
C3—C4—H4	120.1	H15A—C15—H15C	109.5
N1—C5—C4	124.0 (5)	H15B—C15—H15C	109.5
N1—C5—H5A	118.0	O4—C16—O3	124.2 (6)
C4—C5—H5A	118.0	O4—C16—C17	121.5 (7)
C7—C6—C3	117.7 (5)	O3—C16—C17	114.4 (7)
C7—C6—H6A	107.9	C16—C17—H17A	109.5
C3—C6—H6A	107.9	C16—C17—H17B	109.5
C7—C6—H6B	107.9	H17A—C17—H17B	109.5
C3—C6—H6B	107.9	C16—C17—H17C	109.5
H6A—C6—H6B	107.2	H17A—C17—H17C	109.5
C6—C7—C8	113.1 (5)	H17B—C17—H17C	109.5
C6—C7—H7A	109.0	Cu1—O5—H1W	80.8
C8—C7—H7A	109.0	Cu1—O5—H2W	159.1
C6—C7—H7B	109.0	H1W—O5—H2W	111.2
C8—C7—H7B	109.0	H3W—O6—H4W	129.1

O3—Cu1—O1—C14	156.8 (13)	C1—N1—C5—C4	0.4 (8)
N1—Cu1—O1—C14	−100.8 (5)	Cu1—N1—C5—C4	178.0 (5)
N2^{i}—Cu1—O1—C14	87.1 (5)	C3—C4—C5—N1	0.5 (9)
O5—Cu1—O1—C14	−11.0 (5)	C2—C3—C6—C7	−174.9 (5)

O1—Cu1—O3—C16	12.0 (17)	C4—C3—C6—C7	3.6 (8)
N1—Cu1—O3—C16	−90.4 (4)	C3—C6—C7—C8	170.5 (5)
N2^{i}—Cu1—O3—C16	81.8 (4)	C6—C7—C8—C9	66.6 (7)
O5—Cu1—O3—C16	180.0 (4)	C7—C8—C9—C10	47.2 (8)
O3—Cu1—N1—C5	−36.9 (4)	C7—C8—C9—C13	−134.2 (6)
O1—Cu1—N1—C5	150.1 (4)	C13—C9—C10—C11	−2.7 (8)
N2^{i}—Cu1—N1—C5	−116.2 (13)	C8—C9—C10—C11	175.9 (5)
O5—Cu1—N1—C5	53.1 (4)	C12—N2—C11—C10	0.9 (9)
O3—Cu1—N1—C1	140.5 (4)	Cu1^{ii}—N2—C11—C10	177.5 (4)
O1—Cu1—N1—C1	−32.6 (4)	C9—C10—C11—N2	0.9 (9)
N2^{i}—Cu1—N1—C1	61.1 (15)	C11—N2—C12—C13	−0.8 (9)
O5—Cu1—N1—C1	−129.5 (4)	Cu1^{ii}—N2—C12—C13	−177.4 (5)
C5—N1—C1—C2	−1.3 (8)	N2—C12—C13—C9	−0.9 (10)
Cu1—N1—C1—C2	−178.8 (4)	C10—C9—C13—C12	2.7 (8)
N1—C1—C2—C3	1.3 (9)	C8—C9—C13—C12	−176.0 (6)
C1—C2—C3—C4	−0.2 (8)	Cu1—O1—C14—O2	10.7 (9)
C1—C2—C3—C6	178.4 (5)	Cu1—O1—C14—C15	−169.1 (4)
C2—C3—C4—C5	−0.6 (8)	Cu1—O3—C16—O4	6.4 (7)
C6—C3—C4—C5	−179.2 (5)	Cu1—O3—C16—C17	−174.7 (4)

Symmetry codes: (i) −*x*+7/4, *y*−1/4, *z*−3/4; (ii) −*x*+7/4, *y*+1/4, *z*+3/4.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H1W···O2	0.83	1.96	2.663 (8)	142
O5—H2W···O6^{iii}	0.83	1.99	2.795 (8)	164
O6—H3W···O4	0.83	1.96	2.730 (7)	154
O6—H4W···O1^{iv}	0.85	2.07	2.916 (7)	180

Symmetry codes: (iii) −*x*+7/4, *y*+1/4, *z*−1/4; (iv) *x*−1/4, −*y*+1/4, *z*−1/4.

Fig. 1

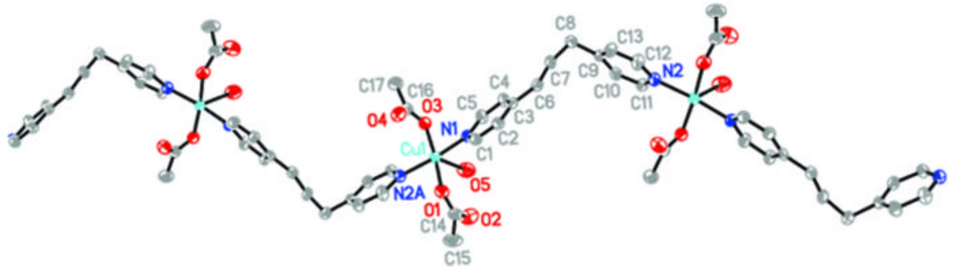
C17
C16
O3
O4
C5
C4
N1
Cu1
C3
C2
C1
C6
C7
C8
C13
C12
C9
N2
C10
C11
O5
N2A
O1
C14
O2
C15

Fig. 2