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catena-Poly[[[bis(glycolato-κ^2O,O')copper(II)]-μ-4,4′-bipyridine-$\kappa^2N:N'$] ethane-1,2-diol monosolvate]

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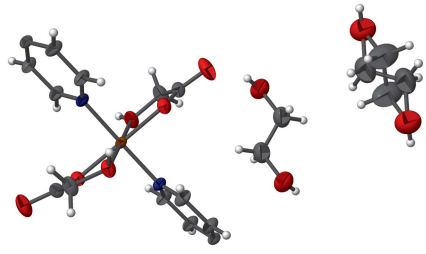
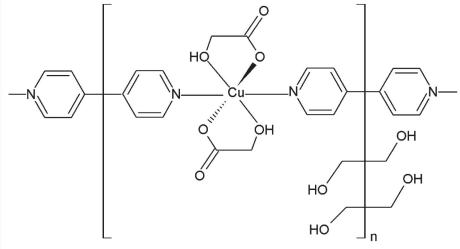
In the title compound, $\{[Cu(C_2H_3O_3)_2(C_{10}H_8N_2)]\cdot C_2H_6O_2\}_n$, the Cu^{II} cation is six-coordinated in a slightly distorted octahedral manner by two N atoms from two different bridging 4,4′-bipyridine (4,4′-bipy) ligands and four O atoms from two individual glycolate anions. The 4,4′-bipy ligand bridges adjacent Cu^{II} centres, generating linear chains running parallel to the $[1\bar{1}0]$ direction. In the crystal structure, adjacent chains are further connected by classical O—H···O hydrogen bonds, resulting in a two-dimensional supermolecular network structure parallel to (100). The C atom of one of the ethane-1,2-diol solvent molecules is disordered over two sets of sites with occupancies of 0.51 (2) and 0.49 (2).

3D view



Chemical scheme



Structure description

In recent years, the self-assembly of coordination polymers and the crystal engineering of metal-organic coordination frameworks have attracted great interest, owing to their intriguing structures and potential application as functional materials (Pan *et al.*, 2004; Zhong, 2014; Xu *et al.*, 2017). Much research has been carried out based on using mixed N- and O-donor ligands to construct metal-organic framework materials (Luo *et al.*, 2012; Moulton & Zaworotko, 2001). 4,4′-Bipyridine (4,4′-bipy) is widely used as a bridging ligand in the construction of coordination polymers. Many copper complexes with polycarboxylic acid and 4,4′-bipy, such as *catena*-[tetrakis(μ_4-*trans*-cyclohexane-1,4-dicarboxylato)bis(μ_2-4,4′-bipyridyl)dicopper(II) *trans*-cyclohexane-1,4-dicarboxyic acid hydrate] (Chen *et al.*, 2006), *catena*-[bis(μ_2-(1*R*,2*R*)-1,2-cyclohexanedicarboxylato)bis-(μ_2-(1*R*,2*R*)-hydrogen 1,2-cyclohexanedicarboxylato)tris(μ^2-4,4′-bipyridine)tricopper tetrahydrate] (Yue *et al.*, 2016), *catena*-[bis(μ_3-isophthalato)bis(μ_2-4,4′-bipyridyl)di-

Table 1
Selected geometric parameters (Å, °).

Cu1—O4	1.9875 (13)	Cu1—N1	2.0159 (14)
Cu1—O2	1.9902 (12)	Cu1—O5	2.2979 (13)
Cu1—N2	2.0100 (14)	Cu1—O1	2.3177 (13)
O4—Cu1—N2	88.91 (6)	N2—Cu1—O5	90.18 (6)
O2—Cu1—N2	91.55 (6)	N1—Cu1—O5	89.15 (6)
O4—Cu1—N1	90.61 (6)	N2—Cu1—O1	89.97 (5)
O2—Cu1—N1	88.92 (6)	N1—Cu1—O1	90.71 (6)
N2—Cu1—N1	179.25 (6)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O6^{i}	0.82	1.88	2.6412 (19)	153
O5—H5···O3^{ii}	0.82	1.84	2.6307 (19)	161
O7—H7···O6	0.82	1.98	2.769 (2)	160
O8—H8···O3^{iii}	0.82	2.23	2.799 (3)	126

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

copper(II) hexahydrate] (Wen *et al.*, 2005), or *catena*-[(μ_6-benzene-1,2,4,5-tetracarboxylato)bis(μ_4-benzene-1,2,4-tricarboxylato-5-carboxylic acid)bis(4,4′-bipyridinium)tetraaquatetracopper(II) tetrahydrate] (Cao *et al.*, 2002) have been synthesized and reported. The crystal structure has not been reported previously.

The title compound crystallizes in the monoclinic space group $P\overline{1}$. The asymmetric unit consists of one Cu^{II} ion, two half 4,4′-bipyridine molecules, two glycolate anions and two half non-coordinating ethane-1,2-diol molecules. As shown in Fig. 1, the Cu^{II} cation is coordinated by two N atoms (N1 and N2) of two bridging 4,4′-bipy ligands occupying the axial positions and four O atoms (O1, O2, O4 and O5) of two different glycolate anions occupying the equatorial sites, forming a distorted octahedral CuN_2O_4 coordination sphere. Atoms Cu1, O1, O2, O4, O5 are almost coplanar, the mean deviation from the plane being 0.003 Å. The *cis* bond angles around the Cu^{II} cation are in the range 88.91 (6)–91.55 (6)° (Fig. 1). The Cu—O bonds involving the carboxyl groups are considerably longer [2.2979 (13) – 2.3177 (13) Å] than those to

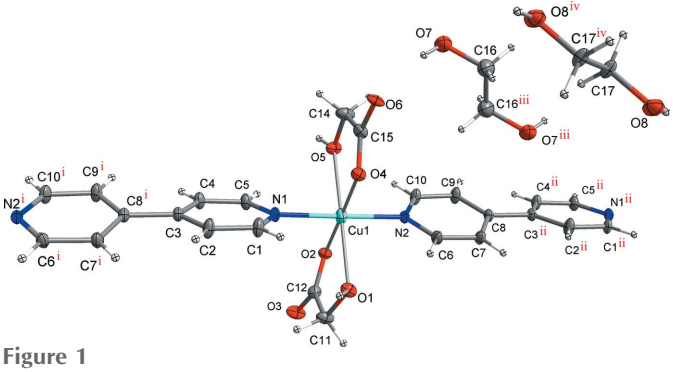


Figure 1
The expanded asymmetric unit of the title complex showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i) $-x+1, -y+1, z$; (ii) $-x+1, y+1, z$; (iii) $-x+1, -y+1, -z+1$.]

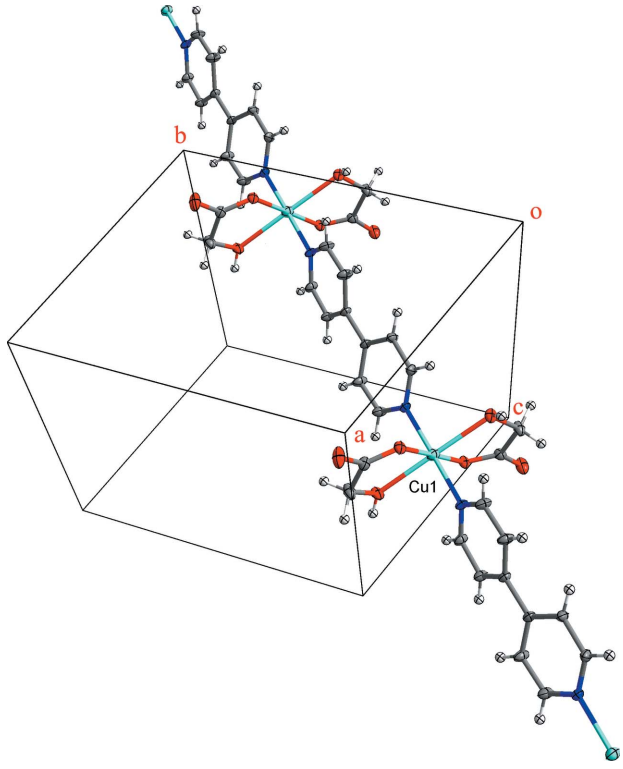


Figure 2
One-dimensional structure of the title polymer constructed by 4,4′-bipy ligands bridging the Cu^{II} ions along the [1$\overline{1}$0] direction. The solvate ethane-1,2-diol molecules have been omitted for clarity.

the hydroxyl group [1.9875 (13) – 1.9902 (12) Å] (Fig. 1 and Table 1). The two O—Cu—O bite angles are 76.16 (5) and 76.72 (5)°. The Cu—N bond lengths vary from 2.0100 (14) to 2.0159 (14) Å, comparable with that observed in the methyl-substituted glycolate-copper compound [2.049 (2) Å; Carballo

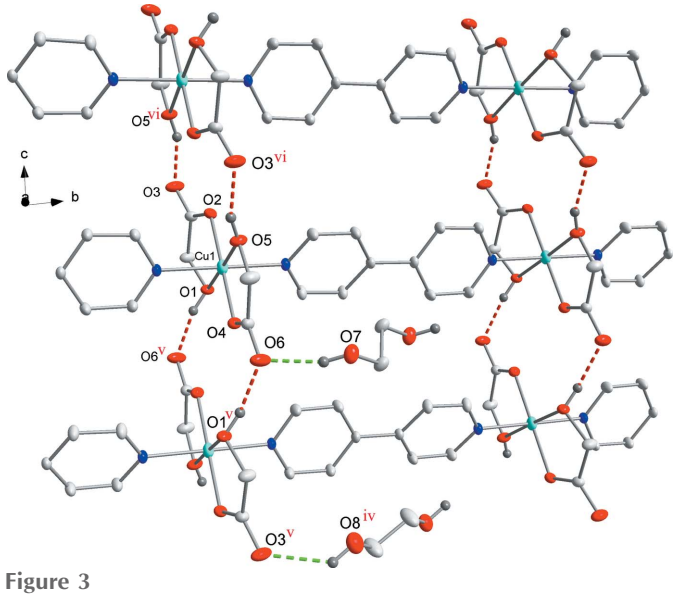


Figure 3
Two-dimensional supramolecular structure of the title polymer, formed by O—H···O hydrogen bonds [shown as red or green dashed lines; symmetry codes: (iv) $-x+1, -y+1, -z$; (v) $-x+1, -y, -z+1$; (vi) $-x+1, -y, -z+2$].

et al., 2001]. The two pyridine rings of the 4,4′-bipyridine unit are twisted slightly away from each other, forming a dihedral angle of 14.15 (13)°. The two non-coordinating ethane-1,2-diol molecules lie on inversion centres (Fig. 1). The bridging 4,4′-bipy ligands link the Cu^{II} cations, giving rise to infinite chains along the [1$\bar{1}$0] direction (Fig. 2).

In the crystal, neighbouring chains are further connected by $O_{hydroxyl}$—H···$O_{carboxyl}$ (O1—H1···O6^{i} and O5—H3···O3^{ii}) hydrogen bonds (Table 2), resulting in a two-dimensional supramolecular structure running parallel to the (100) plane (Fig. 3). The solvent ethane-1,2-diol molecules reside in this layer and are linked to the complex molecules via classical O7—H7···O6 and O8—H8···O3^{iii} hydrogen-bonding interactions (Fig. 3 and Table 2).

Synthesis and crystallization

0.10 mmol of $CuSO_4{\cdot}5H_2O$, 0.10 mmol of 4,4′-bipyridine, 0.10 mmol of sodium glycolate, 0.10 mmol of cyclohexane-1,3,5-tricarboxylate, 9 ml of water and 3 ml of ethane-1,2-diol were mixed and placed in a thick Pyrex tube, which was sealed and heated to 403 K for 72 h. The tube was cooled to ambient temperature spontaneously, whereupon blue block-shaped crystals (37% yield, base on Cu) suitable for X-ray analysis were obtained.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. One solvent ethane-1,2-diol molecular (atom C17) is disordered over two sets of sites with occupancies of 0.51 (2) and 0.49 (2).

Table 3
Experimental details.

Crystal data	
Chemical formula	$[Cu(C_{10}H_8N_2)(C_2H_3O_3)_2]{\cdot}C_2H_6O_2$
M_r	431.88
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	293
a, b, c (Å)	8.0214 (8), 11.0562 (11), 11.2503 (11)
α, β, γ (°)	84.437 (4), 77.592 (4), 69.037 (4)
V (Å^3)	909.72 (16)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.25
Crystal size (mm)	0.30 × 0.25 × 0.22
Data collection	
Diffractometer	Rigaku Mercury CCD
Absorption correction	Multi-scan (*REQAB*; Rigaku, 1998)
T_{min}, T_{max}	0.715, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	32734, 4538, 4002
R_{int}	0.045
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.669
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.030, 0.080, 1.04
No. of reflections	4538
No. of parameters	254
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.43, −0.37

Computer programs: *CrystalClear* (Rigaku, 2007), *XP*, *SHELXTL* and *SHELXS* (Sheldrick, 2008) and *SHELXL* (Sheldrick, 2015).

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References

Cao, R., Shi, Q., Sun, D., Hong, M. C., Bi, W. H. & Zhao, Y. J. (2002). *Inorg. Chem.* **41**, 6161–6168.
Carballo, R., Castiñeiras, A., Covelo, B. & Vázquez-López, E. M. (2001). *Polyhedron*, **20**, 899–904.
Chen, B., Fronczek, F. R., Courtney, B. H. & Zapata, F. (2006). *Cryst. Growth Des.* **6**, 825–828.
Luo, L., Zhao, Y., Lu, Y., Okamura, T. & Sun, W.-Y. (2012). *Polyhedron*, **38**, 88–96.
Moulton, B. & Zaworotko, M. J. (2001). *Chem. Rev.* **101**, 1629–1658.
Pan, L., Sander, M.-B., Huang, X.-Y., Li, J., Smith, M., Bittner, E., Bockrath, B. & Johnson, J.-K. (2004). *J. Am. Chem. Soc.* **126**, 1308–1309.
Rigaku (1998). *REQAB*. Molecular Structure Corporation, The Woodlands, Texas, USA.
Rigaku (2007). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
Wen, Y.-H., Cheng, J.-K., Feng, Y.-L., Zhang, J., Li, Z.-J. & Yao, Y.-G. (2005). *Inorg. Chim. Acta*, **358**, 3347–3354.
Xu, W., Si, Z.-X., Xie, M., Zhou, L.-X. & Zheng, Y.-Q. (2017). *Cryst. Growth Des.* **17**, 2147–2157.
Yue, Q., Huang, Q., Gao, Y.-Y. & Gao, E.-Q. (2016). *Inorg. Chim. Acta*, **443**, 110–117.
Zhong, K.-L. (2014). *Acta Cryst.* C**70**, 189–193.

full crystallographic data

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catena-Poly[[[bis(glycolato-κ^2O,O')copper(II)]-μ-4,4′-bipyridine-$\kappa^2N:N'$] ethane-1,2-diol monosolvate]

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***catena*-Poly[[[bis(glycolato-κ^2O,O')copper(II)]-μ-4,4′-bipyridine-$\kappa^2N:N'$] ethane-1,2-diol monosolvate]**

Crystal data

$[Cu(C_2H_3O_3)_2(C_{10}H_8N_2)]\cdot C_2H_6O_2$
M_r = 431.88
Triclinic, $P\overline{1}$
a = 8.0214 (8) Å
b = 11.0562 (11) Å
c = 11.2503 (11) Å
α = 84.437 (4)°
β = 77.592 (4)°
γ = 69.037 (4)°
V = 909.72 (16) Å^3
Z = 2
$F(000)$ = 446
D_x = 1.577 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9717 reflections
θ = 2.7–28.3°
μ = 1.25 mm^{-1}
T = 293 K
Block, blue
0.30 × 0.25 × 0.22 mm

Data collection

Rigaku Mercury CCD diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 28.5714 pixels mm^{-1}
Graphite Monochromator scans
Absorption correction: multi-scan (*REQAB*; Rigaku, 1998)
T_{min} = 0.715, T_{max} = 1.000
32734 measured reflections
4538 independent reflections
4002 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 28.4°, θ_{min} = 2.7°
h = −10→10
k = −14→14
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.080
S = 1.04
4538 reflections
254 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0337P)^2 + 0.6457P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 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.

Refinement. All non-hydrogen atoms were refined anisotropically. The H atoms of 4,4′-bipydine were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). The H atoms of the ethane-1,2-diol and glycolate anion were located in a difference map and then allowed to ride on their parent atoms, with C—H = 0.97 Å and O—H = 0.82 Å; U_{iso}(H) = 1.2U_{eq}(C) and U_{iso}(H) = 1.5U_{eq}(O).

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cu1	0.44924 (3)	0.03560 (2)	0.75186 (2)	0.02006 (7)	
O1	0.23840 (19)	−0.04526 (13)	0.71074 (11)	0.0295 (3)	
H1	0.2736	−0.0927	0.6520	0.044*	
O2	0.32676 (17)	−0.00618 (12)	0.91579 (11)	0.0251 (3)	
O5	0.65660 (18)	0.11466 (14)	0.79711 (11)	0.0318 (3)	
H5	0.7135	0.1032	0.8521	0.048*	
O4	0.57492 (18)	0.07665 (12)	0.58904 (11)	0.0270 (3)	
O7	0.7479 (2)	0.42174 (17)	0.47606 (17)	0.0522 (4)	
H7	0.7709	0.3456	0.4615	0.078*	
O8	0.2632 (3)	0.5987 (2)	0.0048 (2)	0.0690 (6)	
H8	0.1959	0.6602	0.0473	0.103*	
N1	0.63615 (19)	−0.14436 (13)	0.74846 (13)	0.0238 (3)	
N2	0.26552 (19)	0.21599 (13)	0.75465 (13)	0.0235 (3)	
C1	0.6689 (3)	−0.22458 (18)	0.65783 (17)	0.0320 (4)	
H1A	0.6068	−0.1948	0.5939	0.038*	
C2	0.7911 (3)	−0.34969 (18)	0.65555 (17)	0.0327 (4)	
H2A	0.8086	−0.4031	0.5917	0.039*	
C3	0.8882 (2)	−0.39579 (15)	0.74901 (15)	0.0231 (3)	
C4	0.8555 (3)	−0.31038 (17)	0.84135 (17)	0.0296 (4)	
H4A	0.9191	−0.3363	0.9049	0.036*	
C5	0.7288 (3)	−0.18709 (17)	0.83866 (17)	0.0287 (4)	
H5A	0.7071	−0.1318	0.9019	0.034*	
C6	0.1470 (3)	0.25284 (17)	0.67928 (18)	0.0295 (4)	
H6A	0.1485	0.1919	0.6273	0.035*	
C7	0.0230 (2)	0.37657 (17)	0.67491 (18)	0.0289 (4)	
H7A	−0.0575	0.3976	0.6214	0.035*	
C8	0.0191 (2)	0.46982 (15)	0.75130 (15)	0.0228 (3)	
C9	0.1429 (3)	0.43177 (18)	0.82874 (18)	0.0321 (4)	
H9A	0.1460	0.4911	0.8807	0.038*	
C10	0.2614 (3)	0.30553 (18)	0.82819 (18)	0.0316 (4)	
H10A	0.3423	0.2815	0.8815	0.038*	
C11	0.1822 (3)	−0.1122 (2)	0.81534 (16)	0.0333 (4)	
H11A	0.2350	−0.2046	0.8015	0.040*	
H11B	0.0508	−0.0880	0.8307	0.040*	
C12	0.2392 (2)	−0.08201 (18)	0.92580 (15)	0.0262 (4)	
O3	0.1938 (2)	−0.13645 (16)	1.02335 (12)	0.0426 (4)	
C14	0.7542 (3)	0.1516 (2)	0.69024 (18)	0.0386 (5)	
H14A	0.8828	0.1021	0.6840	0.046*	
H14B	0.7378	0.2426	0.6937	0.046*	
C15	0.6921 (3)	0.12971 (17)	0.57861 (16)	0.0270 (4)	

O6	0.7644 (2)	0.16704 (16)	0.47915 (13)	0.0460 (4)	
C16	0.5753 (3)	0.4975 (3)	0.4482 (2)	0.0553 (6)	
H16A	0.5575	0.4612	0.3789	0.066*	
H16B	0.5734	0.5849	0.4258	0.066*	
C17	0.4363 (15)	0.5519 (12)	0.0376 (16)	0.086 (4)	0.49 (2)
H17A	0.4236	0.5217	0.1219	0.103*	0.49 (2)
H17B	0.4832	0.6223	0.0311	0.103*	0.49 (2)
C17′	0.4585 (12)	0.5495 (10)	−0.0389 (15)	0.079 (4)	0.51 (2)
H17C	0.4853	0.5165	−0.1203	0.095*	0.51 (2)
H17D	0.5065	0.6191	−0.0429	0.095*	0.51 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.01994 (11)	0.01348 (10)	0.02389 (11)	−0.00219 (7)	−0.00471 (7)	0.00000 (7)
O1	0.0425 (7)	0.0317 (7)	0.0197 (6)	−0.0182 (6)	−0.0074 (5)	−0.0014 (5)
O2	0.0295 (6)	0.0273 (6)	0.0215 (6)	−0.0127 (5)	−0.0047 (5)	−0.0038 (5)
O5	0.0365 (7)	0.0453 (8)	0.0219 (6)	−0.0219 (6)	−0.0114 (5)	0.0039 (5)
O4	0.0334 (7)	0.0296 (6)	0.0225 (6)	−0.0149 (5)	−0.0079 (5)	−0.0003 (5)
O7	0.0435 (9)	0.0453 (9)	0.0752 (12)	−0.0208 (8)	−0.0207 (8)	0.0067 (8)
O8	0.0593 (12)	0.0620 (12)	0.0925 (16)	−0.0278 (10)	−0.0131 (11)	−0.0111 (11)
N1	0.0249 (7)	0.0159 (6)	0.0259 (7)	−0.0007 (5)	−0.0060 (6)	−0.0011 (5)
N2	0.0222 (7)	0.0169 (6)	0.0287 (7)	−0.0028 (5)	−0.0063 (6)	−0.0007 (5)
C1	0.0353 (10)	0.0252 (9)	0.0284 (9)	0.0030 (7)	−0.0140 (8)	−0.0032 (7)
C2	0.0361 (10)	0.0247 (9)	0.0301 (9)	0.0044 (8)	−0.0135 (8)	−0.0089 (7)
C3	0.0226 (8)	0.0164 (7)	0.0266 (8)	−0.0018 (6)	−0.0053 (6)	−0.0005 (6)
C4	0.0349 (10)	0.0212 (8)	0.0295 (9)	−0.0002 (7)	−0.0148 (7)	−0.0029 (7)
C5	0.0349 (10)	0.0196 (8)	0.0283 (9)	−0.0020 (7)	−0.0101 (7)	−0.0046 (7)
C6	0.0304 (9)	0.0183 (8)	0.0420 (10)	−0.0051 (7)	−0.0156 (8)	−0.0043 (7)
C7	0.0290 (9)	0.0198 (8)	0.0387 (10)	−0.0035 (7)	−0.0164 (8)	−0.0025 (7)
C8	0.0220 (8)	0.0173 (7)	0.0254 (8)	−0.0020 (6)	−0.0047 (6)	−0.0013 (6)
C9	0.0367 (10)	0.0221 (8)	0.0333 (10)	0.0014 (7)	−0.0154 (8)	−0.0079 (7)
C10	0.0336 (10)	0.0245 (9)	0.0326 (9)	0.0018 (7)	−0.0162 (8)	−0.0055 (7)
C11	0.0450 (11)	0.0433 (11)	0.0234 (8)	−0.0277 (9)	−0.0104 (8)	0.0014 (8)
C12	0.0289 (9)	0.0303 (9)	0.0208 (8)	−0.0110 (7)	−0.0053 (7)	−0.0022 (7)
O3	0.0612 (10)	0.0599 (10)	0.0236 (7)	−0.0408 (8)	−0.0121 (6)	0.0073 (6)
C14	0.0477 (12)	0.0560 (13)	0.0272 (9)	−0.0349 (11)	−0.0122 (8)	0.0053 (9)
C15	0.0348 (9)	0.0253 (8)	0.0227 (8)	−0.0125 (7)	−0.0058 (7)	−0.0008 (6)
O6	0.0736 (11)	0.0574 (10)	0.0233 (7)	−0.0460 (9)	−0.0029 (7)	−0.0004 (6)
C16	0.0518 (15)	0.0618 (16)	0.0547 (15)	−0.0237 (13)	−0.0163 (12)	0.0167 (13)
C17	0.082 (6)	0.093 (7)	0.076 (8)	−0.004 (5)	−0.032 (5)	−0.033 (5)
C17′	0.080 (6)	0.079 (6)	0.078 (8)	−0.039 (5)	−0.008 (5)	0.021 (5)

Geometric parameters (Å, º)

Cu1—O4	1.9875 (13)	C4—H4A	0.9300
Cu1—O2	1.9902 (12)	C5—H5A	0.9300
Cu1—N2	2.0100 (14)	C6—C7	1.378 (2)

Cu1—N1	2.0159 (14)	C6—H6A	0.9300
Cu1—O5	2.2979 (13)	C7—C8	1.393 (2)
Cu1—O1	2.3177 (13)	C7—H7A	0.9300
O1—C11	1.406 (2)	C8—C9	1.387 (2)
O1—H1	0.8200	C8—C3^{ii}	1.483 (2)
O2—C12	1.256 (2)	C9—C10	1.379 (2)
O5—C14	1.398 (2)	C9—H9A	0.9300
O5—H5	0.8200	C10—H10A	0.9300
O4—C15	1.255 (2)	C11—C12	1.516 (2)
O7—C16	1.422 (3)	C11—H11A	0.9700
O7—H7	0.8200	C11—H11B	0.9700
O8—C17	1.415 (9)	C12—O3	1.248 (2)
O8—C17′	1.451 (9)	C14—C15	1.516 (2)
O8—H8	0.8200	C14—H14A	0.9700
N1—C5	1.336 (2)	C14—H14B	0.9700
N1—C1	1.337 (2)	C15—O6	1.250 (2)
N2—C10	1.338 (2)	C16—C16^{iii}	1.476 (5)
N2—C6	1.338 (2)	C16—H16A	0.9700
C1—C2	1.379 (2)	C16—H16B	0.9700
C1—H1A	0.9300	C17—C17^{iv}	1.43 (2)
C2—C3	1.391 (2)	C17—H17A	0.9700
C2—H2A	0.9300	C17—H17B	0.9700
C3—C4	1.391 (2)	C17′—C17′^{iv}	1.40 (2)
C3—C8^{i}	1.483 (2)	C17′—H17C	0.9700
C4—C5	1.381 (2)	C17′—H17D	0.9700

O4—Cu1—O2	179.17 (5)	C6—C7—C8	119.43 (16)
O4—Cu1—N2	88.91 (6)	C6—C7—H7A	120.3
O2—Cu1—N2	91.55 (6)	C8—C7—H7A	120.3
O4—Cu1—N1	90.61 (6)	C9—C8—C7	117.25 (15)
O2—Cu1—N1	88.92 (6)	C9—C8—C3^{ii}	121.67 (15)
N2—Cu1—N1	179.25 (6)	C7—C8—C3^{ii}	121.08 (15)
O4—Cu1—O5	76.72 (5)	C10—C9—C8	119.63 (17)
O2—Cu1—O5	102.58 (5)	C10—C9—H9A	120.2
N2—Cu1—O5	90.18 (6)	C8—C9—H9A	120.2
N1—Cu1—O5	89.15 (6)	N2—C10—C9	123.16 (17)
O4—Cu1—O1	104.54 (5)	N2—C10—H10A	118.4
O2—Cu1—O1	76.16 (5)	C9—C10—H10A	118.4
N2—Cu1—O1	89.97 (5)	O1—C11—C12	111.44 (15)
N1—Cu1—O1	90.71 (6)	O1—C11—H11A	109.3
O5—Cu1—O1	178.73 (4)	C12—C11—H11A	109.3
C11—O1—Cu1	108.23 (10)	O1—C11—H11B	109.3
C11—O1—H1	109.5	C12—C11—H11B	109.3
Cu1—O1—H1	115.5	H11A—C11—H11B	108.0
C12—O2—Cu1	119.71 (11)	O3—C12—O2	123.92 (16)
C14—O5—Cu1	110.19 (10)	O3—C12—C11	115.97 (16)
C14—O5—H5	109.5	O2—C12—C11	120.11 (15)
Cu1—O5—H5	135.7	O5—C14—C15	111.50 (15)

C15—O4—Cu1	121.09 (11)	O5—C14—H14A	109.3
C16—O7—H7	109.5	C15—C14—H14A	109.3
C17—O8—H8	109.5	O5—C14—H14B	109.3
C5—N1—C1	118.29 (15)	C15—C14—H14B	109.3
C5—N1—Cu1	120.32 (12)	H14A—C14—H14B	108.0
C1—N1—Cu1	121.38 (12)	O6—C15—O4	123.69 (16)
C10—N2—C6	117.25 (15)	O6—C15—C14	116.06 (16)
C10—N2—Cu1	121.50 (12)	O4—C15—C14	120.25 (16)
C6—N2—Cu1	121.19 (12)	O7—C16—C16^{iii}	112.2 (3)
N1—C1—C2	122.55 (17)	O7—C16—H16A	109.2
N1—C1—H1A	118.7	C16^{iii}—C16—H16A	109.2
C2—C1—H1A	118.7	O7—C16—H16B	109.2
C1—C2—C3	119.85 (17)	C16^{iii}—C16—H16B	109.2
C1—C2—H2A	120.1	H16A—C16—H16B	107.9
C3—C2—H2A	120.1	O8—C17—C17^{iv}	112.3 (9)
C2—C3—C4	116.96 (15)	O8—C17—H17A	109.1
C2—C3—C8^{i}	121.75 (15)	C17^{iv}—C17—H17A	109.1
C4—C3—C8^{i}	121.29 (15)	O8—C17—H17B	109.1
C5—C4—C3	119.97 (16)	C17^{iv}—C17—H17B	109.1
C5—C4—H4A	120.0	H17A—C17—H17B	107.9
C3—C4—H4A	120.0	C17′^{iv}—C17′—O8	110.1 (10)
N1—C5—C4	122.35 (16)	C17′^{iv}—C17′—H17C	109.6
N1—C5—H5A	118.8	O8—C17′—H17C	109.6
C4—C5—H5A	118.8	C17′^{iv}—C17′—H17D	109.6
N2—C6—C7	123.27 (16)	O8—C17′—H17D	109.6
N2—C6—H6A	118.4	H17C—C17′—H17D	108.2
C7—C6—H6A	118.4		

C5—N1—C1—C2	1.4 (3)	C7—C8—C9—C10	−0.7 (3)
Cu1—N1—C1—C2	−177.56 (16)	C3^{ii}—C8—C9—C10	179.62 (18)
N1—C1—C2—C3	−1.2 (3)	C6—N2—C10—C9	−0.4 (3)
C1—C2—C3—C4	−0.2 (3)	Cu1—N2—C10—C9	176.97 (16)
C1—C2—C3—C8^{i}	179.14 (18)	C8—C9—C10—N2	0.9 (3)
C2—C3—C4—C5	1.3 (3)	Cu1—O1—C11—C12	13.88 (19)
C8^{i}—C3—C4—C5	−178.03 (17)	Cu1—O2—C12—O3	163.10 (15)
C1—N1—C5—C4	−0.2 (3)	Cu1—O2—C12—C11	−16.9 (2)
Cu1—N1—C5—C4	178.76 (15)	O1—C11—C12—O3	179.47 (17)
C3—C4—C5—N1	−1.2 (3)	O1—C11—C12—O2	−0.5 (3)
C10—N2—C6—C7	−0.3 (3)	Cu1—O5—C14—C15	0.6 (2)
Cu1—N2—C6—C7	−177.66 (15)	Cu1—O4—C15—O6	−174.01 (15)
N2—C6—C7—C8	0.5 (3)	Cu1—O4—C15—C14	6.1 (2)
C6—C7—C8—C9	0.0 (3)	O5—C14—C15—O6	175.96 (18)
C6—C7—C8—C3^{ii}	179.75 (17)	O5—C14—C15—O4	−4.2 (3)

Symmetry codes: (i) *x*+1, *y*−1, *z*; (ii) *x*−1, *y*+1, *z*; (iii) −*x*+1, −*y*+1, −*z*+1; (iv) −*x*+1, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O6^{v}	0.82	1.88	2.6412 (19)	153
O5—H5···O3^{vi}	0.82	1.84	2.6307 (19)	161
O7—H7···O6	0.82	1.98	2.769 (2)	160
O8—H8···O3^{vii}	0.82	2.23	2.799 (3)	126

Symmetry codes: (v) −*x*+1, −*y*, −*z*+1; (vi) −*x*+1, −*y*, −*z*+2; (vii) *x*, *y*+1, *z*−1.