Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[[diaquabis{μ-4-[6-(4-carboxyphenyl)-4,4′-bipyridin-2-yl]benzoato-κ^2O:$N^{1'}$}copper(II)] dimethylformamide tetrasolvate]

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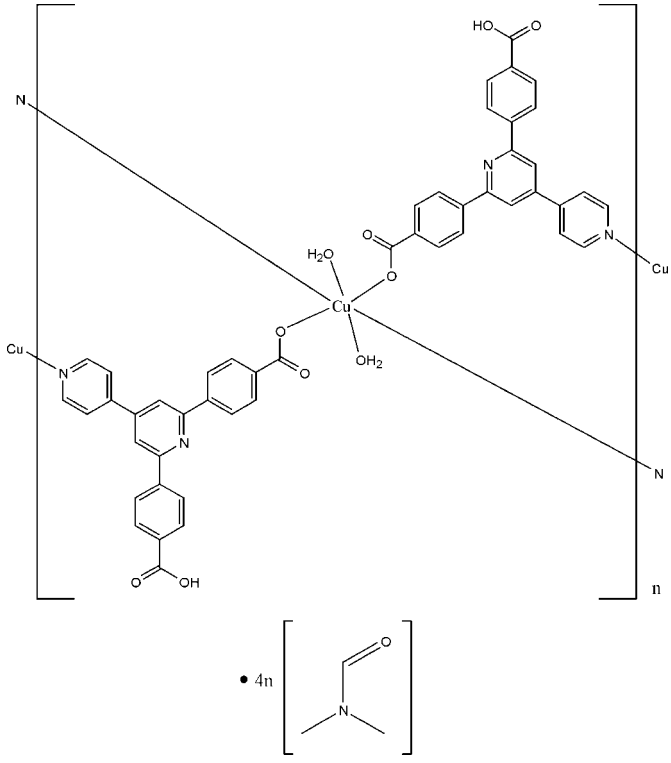
Received 28 February 2013; accepted 6 March 2013

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.061; wR factor = 0.185; data-to-parameter ratio = 13.9.

In the title compound, $\{[Cu(C_{24}H_{15}N_2O_4)_2(H_2O)_2]\cdot 4C_3H_7NO\}_n$, the Cu^{II} ion, lying on an inversion center, is six-coordinated by two N atoms from two 4-[6-(4-carboxyphenyl)-4,4′-bipyridin-2-yl]benzoate (L) ligands, two deprotonated carboxylate O atoms from two other symmetry-related L ligands and two water molecules in a slightly distorted octahedral geometry. The Cu^{II} atoms are linked by the bridging ligands into a layer parallel to (101). The presence of intralayer O—H···O hydrogen bonds and π–π interactions between the pyridine and benzene rings [centroid–centroid distances = 3.808 (2) and 3.927 (2) Å] stabilizes the layer. Further O—H···O hydrogen bonds link the layers and the dimethylformamide solvent molecules.

Related literature

For the design of metal-organic coordination polymers, see: Ge & Song (2012); Herm *et al.* (2011); Liu *et al.* (2010); Wang *et al.* (2010). For a related structure, see: Xia *et al.* (2012).



Experimental

Crystal data

$[Cu(C_{24}H_{15}N_2O_4)_2(H_2O)_2]\cdot 4C_3H_7NO$
M_r = 1182.73
Monoclinic, $P2_1/n$
a = 7.7161 (17) Å
b = 17.550 (4) Å
c = 20.947 (4) Å
β = 96.800 (4)°
V = 2816.6 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.46 mm^{-1}
T = 293 K
0.27 × 0.25 × 0.20 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.885, T_{max} = 0.913
14622 measured reflections
5226 independent reflections
3371 reflections with $I > 2\sigma(I)$
R_{int} = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.185
S = 1.04
5226 reflections
376 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.93 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4A···O2^{i}	0.82	1.86	2.584 (4)	146
O1W—H1A···O5^{ii}	0.85	1.98	2.808 (5)	165
O1W—H1B···O2^{iii}	0.85	1.95	2.758 (4)	159

Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{5}{2}, z-\frac{1}{2}$; (ii) $x+1, y, z$; (iii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve

structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *XP* in *SHELXTL* and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

The authors are grateful for financial aid from The First Hospital of Jilin University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2619).

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supporting information

Acta Cryst. (2013). E**69**, m202–m203 [doi:10.1107/S1600536813006430]

Poly[[diaquabis{μ-4-[6-(4-carboxyphenyl)-4,4′-bipyridin-2-yl]benzoato-κ^2O:$N^{1'}$}copper(II)] dimethylformamide tetrasolvate]

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S1. Comment

Metal-organic coordination polymers (MOCPs) with infinite one-, two- or three-dimensional structures are assembled with metal ions or polynuclear clusters as nodes and organic ligands as linkers (Herm *et al.*, 2011; Liu *et al.*, 2010). Recently, the chemists have devoted themselves to design and synthesize MOCPs, not only due to their potential applications in the realm of gas adsorption and separation, catalysis, magnetism, luminescence, host–guest chemistry and *etc*, but also for their aesthetic and often complicated architectures and topologies (Ge & Song, 2012; Wang *et al.*, 2010). In order to extend the investigations in this field, we used a multifunctional ligand, 4,4′-(4,4′-bipyridine-2,6-diyl)di-benzoic acid ($bpydbH_2$) to design and synthesize the title copper(II) complex and report its structure here.

The asymmetric unit of the title compound contains one Cu^{II} ion lying on an inversion center, one anionic bpydbH ligand, one aqua ligand and two lattice DMF molecules. As shown in Fig. 1, the Cu^{II} ion is six-coordinated by two N atoms from two bpydbH ligands, two deprotonated carboxylate O atoms from two other symmetry-related bpydbH ligands and two aqua ligands, furnishing a slightly distorted octahedral geometry. The bond distances and angles are in a normal range (Xia *et al.*, 2012). The Cu nodes are extended by the bridging bpydbH linkers into a layer parallel to (101) (Fig. 2). The presence of intralayer O—H···O hydrogen bonds and π–π interactions between the pyridine and benzene rings [centroid–centroid diatances = 3.808 (2) and 3.927 (2) Å] stabilizes the single layer.

S2. Experimental

$Cu(NO_3)_2.3H_2O$ (0.0063 g, 0.025 mmol) and $bpydbH_2$ (0.0099 g, 0.025 mmol) were suspended in a mixed solvent of di-methylformamide (DMF) (4 ml) and H_2O (0.5 ml), and heated in a 15 ml Teflon-lined stainless-steel autoclave at 80°C for 3 days. After the autoclave was cooled to room temperature slowly, green crystals were collected by filtration and washed with DMF, and dried in air (yield: 65% based on Cu).

S3. Refinement

H atoms on C and carboxyl O atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93, 0.96 and O—H = 0.82 Å and with U_{iso}(H) = 1.2(1.5 for methyl and carboxyl)U_{eq}(C,*O*). H atoms of water molecules were located in a difference Fourier map and refined as riding atoms, with U_{iso}(H) = 1.5U_{eq}(O).

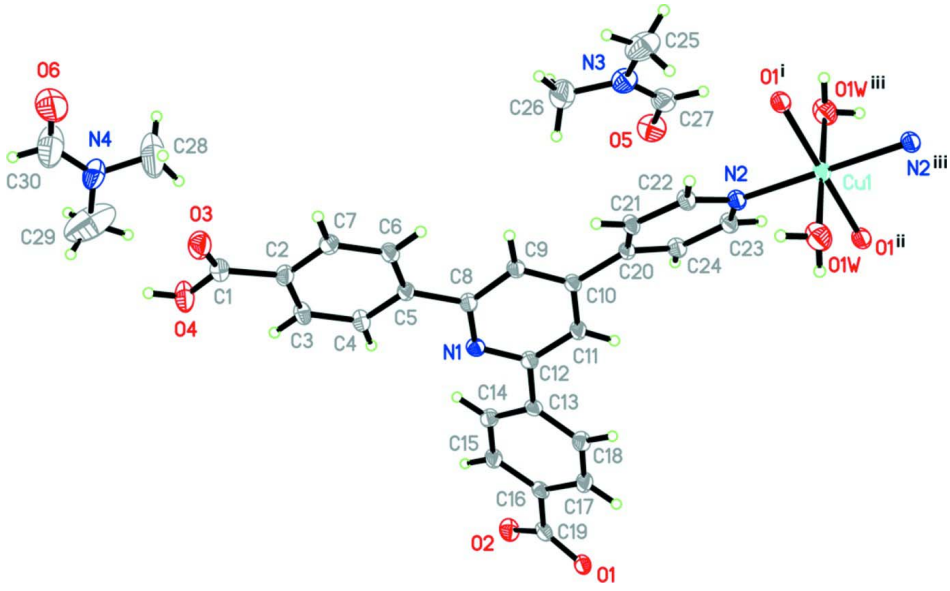

Figure 1

The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i) 1/2 + *x*, 3/2 - *y*, -1/2 + *z*; (ii) 3/2 - *x*, -1/2 + *y*, 1/2 - *z*; (iii) 2 - *x*, 1 - *y*, -*z*.]

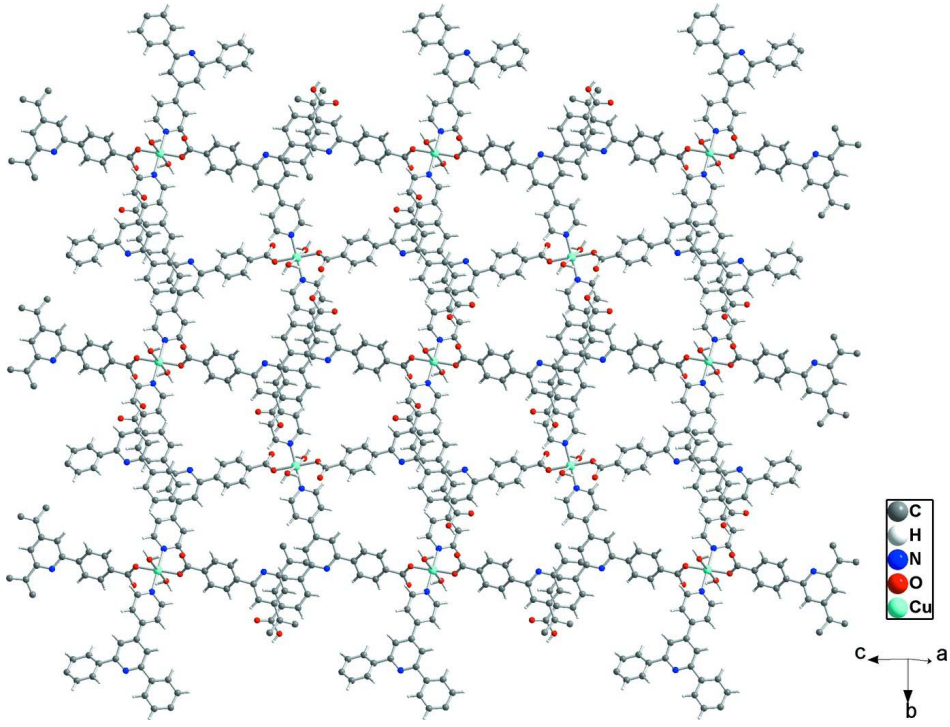

Figure 2

View of the layer structure of the title compound.

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Hall symbol: -P 2yn
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β = 96.800 (4)°
V = 2816.6 (10) Å^3
Z = 2
$F(000)$ = 1238
D_x = 1.395 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5226 reflections
θ = 1.0–26.0°
μ = 0.46 mm^{-1}
T = 293 K
Block, green
0.27 × 0.25 × 0.20 mm

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Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.885, T_{max} = 0.913
14622 measured reflections
5226 independent reflections
3371 reflections with $I > 2\sigma(I)$
R_{int} = 0.058
θ_{max} = 25.5°, θ_{min} = 2.0°
h = −9→7
k = −21→21
l = −20→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.185
S = 1.04
5226 reflections
376 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0891P)^2 + 2.0095P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.93 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
Cu1	1.0000	0.5000	0.0000	0.0362 (2)
C1	0.8452 (6)	1.2336 (2)	−0.1386 (2)	0.0432 (10)
C2	0.8060 (5)	1.1653 (2)	−0.10151 (19)	0.0347 (9)

C3	0.7251 (5)	1.1715 (2)	−0.0455 (2)	0.0369 (10)
H3	0.6854	1.2186	−0.0330	0.044*
C4	0.7040 (5)	1.1079 (2)	−0.0088 (2)	0.0350 (9)
H4	0.6517	1.1128	0.0288	0.042*
C5	0.7592 (5)	1.0363 (2)	−0.02669 (18)	0.0286 (8)
C6	0.8380 (5)	1.0305 (2)	−0.08253 (19)	0.0352 (9)
H6	0.8762	0.9832	−0.0953	0.042*
C7	0.8607 (5)	1.0943 (2)	−0.11976 (19)	0.0376 (10)
H7	0.9132	1.0894	−0.1573	0.045*
C8	0.7389 (5)	0.9695 (2)	0.01565 (19)	0.0302 (8)
C9	0.7683 (5)	0.8950 (2)	−0.00365 (18)	0.0304 (9)
H9	0.7972	0.8853	−0.0447	0.036*
C10	0.7540 (5)	0.83558 (19)	0.03927 (18)	0.0280 (8)
C11	0.7072 (5)	0.8537 (2)	0.09959 (18)	0.0314 (9)
H11	0.6958	0.8154	0.1295	0.038*
C12	0.6774 (5)	0.9291 (2)	0.11507 (18)	0.0299 (8)
C13	0.6253 (5)	0.9511 (2)	0.17864 (18)	0.0301 (9)
C14	0.5242 (5)	1.0156 (2)	0.18392 (19)	0.0358 (9)
H14	0.4924	1.0455	0.1478	0.043*
C15	0.4702 (5)	1.0358 (2)	0.24194 (19)	0.0372 (10)
H15	0.4004	1.0786	0.2445	0.045*
C16	0.5196 (5)	0.9925 (2)	0.29668 (18)	0.0312 (9)
C17	0.6242 (5)	0.9290 (2)	0.29215 (19)	0.0378 (10)
H17	0.6586	0.8998	0.3285	0.045*
C18	0.6777 (5)	0.9089 (2)	0.23352 (19)	0.0366 (9)
H18	0.7494	0.8667	0.2310	0.044*
C19	0.4600 (6)	1.0145 (2)	0.3597 (2)	0.0361 (10)
C20	0.7944 (5)	0.75539 (19)	0.02344 (17)	0.0288 (8)
C21	0.9191 (5)	0.73870 (19)	−0.01677 (18)	0.0307 (9)
H21	0.9689	0.7778	−0.0384	0.037*
C22	0.9695 (5)	0.6647 (2)	−0.02478 (19)	0.0339 (9)
H22	1.0543	0.6549	−0.0517	0.041*
C23	0.7732 (5)	0.6214 (2)	0.04100 (19)	0.0360 (9)
H23	0.7197	0.5811	0.0598	0.043*
C24	0.7177 (5)	0.6942 (2)	0.05158 (18)	0.0342 (9)
H24	0.6294	0.7025	0.0774	0.041*
C25	0.6692 (8)	0.6406 (4)	−0.1720 (3)	0.0829 (19)
H25A	0.7059	0.6773	−0.2016	0.124*
H25B	0.6144	0.5984	−0.1955	0.124*
H25C	0.7689	0.6229	−0.1442	0.124*
C26	0.5118 (8)	0.7558 (3)	−0.1443 (3)	0.0756 (16)
H26A	0.5739	0.7741	−0.1783	0.113*
H26B	0.5493	0.7833	−0.1055	0.113*
H26C	0.3889	0.7633	−0.1558	0.113*
C27	0.4770 (6)	0.6364 (3)	−0.0897 (2)	0.0543 (12)
H27	0.5082	0.5854	−0.0843	0.065*
C28	0.4517 (16)	1.2769 (5)	−0.2557 (5)	0.203 (6)
H28A	0.4153	1.2642	−0.2148	0.304*

H28B	0.5656	1.2561	−0.2586	0.304*
H28C	0.3703	1.2562	−0.2895	0.304*
C29	0.4063 (11)	1.3970 (6)	−0.2090 (4)	0.157 (4)
H29A	0.3787	1.3613	−0.1770	0.235*
H29B	0.3054	1.4274	−0.2228	0.235*
H29C	0.4999	1.4294	−0.1912	0.235*
C30	0.5028 (11)	1.3864 (4)	−0.3123 (4)	0.119 (3)
H30	0.4860	1.4387	−0.3166	0.142*
N1	0.6925 (4)	0.98644 (16)	0.07362 (15)	0.0305 (7)
N2	0.9010 (4)	0.60580 (17)	0.00477 (15)	0.0331 (8)
N3	0.5471 (5)	0.6755 (2)	−0.13415 (19)	0.0533 (10)
N4	0.4576 (6)	1.3570 (2)	−0.2622 (2)	0.0619 (11)
O1	0.5313 (4)	0.98064 (14)	0.40897 (13)	0.0395 (7)
O2	0.3418 (4)	1.06386 (16)	0.35908 (14)	0.0488 (8)
O3	0.9397 (5)	1.23445 (17)	−0.18056 (16)	0.0582 (9)
O4	0.7673 (4)	1.29571 (17)	−0.11906 (16)	0.0607 (9)
H4A	0.7916	1.3324	−0.1405	0.091*
O5	0.3740 (4)	0.6624 (2)	−0.05498 (17)	0.0651 (10)
O6	0.5670 (7)	1.3545 (2)	−0.3567 (2)	0.1082 (17)
O1W	1.3019 (4)	0.54357 (17)	0.02770 (15)	0.0552 (8)
H1A	1.3236	0.5847	0.0087	0.083*
H1B	1.2828	0.5552	0.0656	0.083*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0628 (5)	0.0222 (3)	0.0263 (4)	0.0050 (3)	0.0164 (3)	0.0015 (3)
C1	0.054 (3)	0.033 (2)	0.042 (3)	−0.001 (2)	0.005 (2)	0.0034 (19)
C2	0.036 (2)	0.031 (2)	0.037 (2)	−0.0049 (17)	0.0019 (18)	0.0061 (17)
C3	0.040 (2)	0.0251 (19)	0.046 (3)	0.0037 (16)	0.010 (2)	0.0004 (17)
C4	0.039 (2)	0.0273 (19)	0.041 (2)	0.0008 (17)	0.0146 (19)	0.0013 (17)
C5	0.032 (2)	0.0272 (19)	0.027 (2)	−0.0010 (16)	0.0060 (16)	0.0009 (15)
C6	0.048 (2)	0.0254 (18)	0.033 (2)	0.0009 (17)	0.0094 (19)	−0.0029 (16)
C7	0.052 (3)	0.035 (2)	0.028 (2)	−0.0037 (18)	0.0104 (19)	0.0002 (17)
C8	0.034 (2)	0.0256 (18)	0.032 (2)	0.0004 (16)	0.0066 (17)	0.0011 (16)
C9	0.037 (2)	0.0284 (19)	0.027 (2)	0.0006 (16)	0.0088 (17)	−0.0017 (16)
C10	0.033 (2)	0.0240 (18)	0.028 (2)	−0.0001 (15)	0.0067 (16)	−0.0014 (15)
C11	0.042 (2)	0.0257 (19)	0.027 (2)	0.0008 (16)	0.0090 (17)	0.0019 (16)
C12	0.036 (2)	0.0275 (19)	0.027 (2)	−0.0004 (16)	0.0085 (17)	0.0000 (16)
C13	0.038 (2)	0.0284 (19)	0.025 (2)	−0.0028 (16)	0.0074 (17)	−0.0047 (15)
C14	0.048 (2)	0.033 (2)	0.027 (2)	0.0025 (17)	0.0097 (19)	0.0007 (16)
C15	0.050 (2)	0.030 (2)	0.034 (2)	0.0050 (18)	0.0104 (19)	−0.0020 (17)
C16	0.041 (2)	0.0259 (19)	0.029 (2)	−0.0039 (16)	0.0126 (17)	−0.0045 (16)
C17	0.051 (3)	0.032 (2)	0.032 (2)	0.0009 (18)	0.0092 (19)	0.0052 (17)
C18	0.047 (2)	0.031 (2)	0.033 (2)	0.0078 (18)	0.0118 (19)	−0.0013 (17)
C19	0.050 (2)	0.026 (2)	0.035 (2)	−0.0054 (18)	0.014 (2)	−0.0043 (17)
C20	0.039 (2)	0.0239 (18)	0.024 (2)	0.0012 (16)	0.0051 (16)	−0.0003 (15)
C21	0.043 (2)	0.0225 (18)	0.029 (2)	−0.0019 (16)	0.0141 (17)	0.0005 (15)

C22	0.047 (2)	0.0275 (19)	0.030 (2)	−0.0006 (17)	0.0146 (18)	−0.0004 (16)
C23	0.052 (3)	0.028 (2)	0.030 (2)	−0.0039 (18)	0.0140 (19)	0.0014 (16)
C24	0.045 (2)	0.031 (2)	0.029 (2)	0.0012 (17)	0.0158 (18)	−0.0017 (16)
C25	0.081 (4)	0.119 (5)	0.052 (4)	0.025 (4)	0.022 (3)	0.004 (3)
C26	0.097 (4)	0.062 (3)	0.069 (4)	−0.003 (3)	0.017 (3)	0.009 (3)
C27	0.056 (3)	0.053 (3)	0.054 (3)	−0.005 (2)	0.005 (3)	−0.002 (2)
C28	0.303 (15)	0.088 (6)	0.196 (11)	−0.064 (8)	−0.057 (10)	0.066 (7)
C29	0.132 (7)	0.259 (12)	0.082 (6)	0.104 (8)	0.025 (5)	0.000 (6)
C30	0.167 (8)	0.079 (5)	0.123 (7)	0.022 (5)	0.067 (6)	0.031 (5)
N1	0.0353 (17)	0.0303 (17)	0.0272 (18)	−0.0014 (13)	0.0090 (14)	−0.0030 (13)
N2	0.049 (2)	0.0260 (16)	0.0265 (18)	0.0009 (14)	0.0128 (15)	0.0000 (13)
N3	0.054 (2)	0.062 (3)	0.046 (2)	0.000 (2)	0.0151 (19)	0.0015 (19)
N4	0.071 (3)	0.059 (3)	0.061 (3)	0.012 (2)	0.027 (2)	0.019 (2)
O1	0.0655 (19)	0.0274 (14)	0.0276 (16)	−0.0003 (13)	0.0135 (14)	−0.0001 (11)
O2	0.071 (2)	0.0377 (16)	0.0413 (19)	0.0105 (15)	0.0232 (15)	−0.0045 (13)
O3	0.082 (2)	0.0458 (19)	0.051 (2)	−0.0038 (17)	0.0217 (19)	0.0064 (15)
O4	0.081 (2)	0.0349 (17)	0.070 (2)	0.0016 (16)	0.0251 (19)	0.0134 (16)
O5	0.060 (2)	0.075 (2)	0.064 (2)	−0.0093 (18)	0.0235 (19)	−0.0012 (19)
O6	0.179 (5)	0.077 (3)	0.083 (3)	−0.005 (3)	0.075 (3)	−0.021 (2)
O1W	0.072 (2)	0.0441 (18)	0.053 (2)	−0.0041 (16)	0.0239 (17)	−0.0006 (15)

Geometric parameters (Å, º)

Cu1—O1^{i}	1.980 (3)	C19—O2	1.256 (5)
Cu1—O1^{ii}	1.980 (3)	C19—O1	1.260 (5)
Cu1—N2	2.015 (3)	C20—C21	1.383 (5)
Cu1—N2^{iii}	2.015 (3)	C20—C24	1.390 (5)
C1—O3	1.207 (5)	C21—C22	1.371 (5)
C1—O4	1.332 (5)	C21—H21	0.9300
C1—C2	1.480 (5)	C22—N2	1.345 (5)
C2—C7	1.383 (5)	C22—H22	0.9300
C2—C3	1.398 (5)	C23—N2	1.342 (5)
C3—C4	1.375 (5)	C23—C24	1.374 (5)
C3—H3	0.9300	C23—H23	0.9300
C4—C5	1.393 (5)	C24—H24	0.9300
C4—H4	0.9300	C25—N3	1.439 (6)
C5—C6	1.385 (5)	C25—H25A	0.9600
C5—C8	1.490 (5)	C25—H25B	0.9600
C6—C7	1.388 (5)	C25—H25C	0.9600
C6—H6	0.9300	C26—N3	1.447 (6)
C7—H7	0.9300	C26—H26A	0.9600
C8—N1	1.340 (5)	C26—H26B	0.9600
C8—C9	1.394 (5)	C26—H26C	0.9600
C9—C10	1.390 (5)	C27—O5	1.226 (5)
C9—H9	0.9300	C27—N3	1.323 (6)
C10—C11	1.392 (5)	C27—H27	0.9300
C10—C20	1.487 (5)	C28—N4	1.413 (9)
C11—C12	1.388 (5)	C28—H28A	0.9600

C11—H11	0.9300	C28—H28B	0.9600
C12—N1	1.343 (5)	C28—H28C	0.9600
C12—C13	1.487 (5)	C29—N4	1.411 (8)
C13—C14	1.385 (5)	C29—H29A	0.9600
C13—C18	1.387 (5)	C29—H29B	0.9600
C14—C15	1.377 (5)	C29—H29C	0.9600
C14—H14	0.9300	C30—O6	1.238 (8)
C15—C16	1.391 (5)	C30—N4	1.255 (7)
C15—H15	0.9300	C30—H30	0.9300
C16—C17	1.385 (5)	O1—Cu1^{iv}	1.980 (3)
C16—C19	1.499 (5)	O4—H4A	0.8200
C17—C18	1.387 (5)	O1W—H1A	0.8501
C17—H17	0.9300	O1W—H1B	0.8489
C18—H18	0.9300		

O1^{i}—Cu1—O1^{ii}	180.0	O2—C19—C16	117.9 (4)
O1^{i}—Cu1—N2	91.16 (11)	O1—C19—C16	116.7 (4)
O1^{ii}—Cu1—N2	88.84 (11)	C21—C20—C24	117.2 (3)
O1^{i}—Cu1—N2^{iii}	88.84 (11)	C21—C20—C10	121.0 (3)
O1^{ii}—Cu1—N2^{iii}	91.16 (11)	C24—C20—C10	121.7 (3)
N2—Cu1—N2^{iii}	180.0	C22—C21—C20	120.2 (3)
O3—C1—O4	123.2 (4)	C22—C21—H21	119.9
O3—C1—C2	124.8 (4)	C20—C21—H21	119.9
O4—C1—C2	112.0 (4)	N2—C22—C21	122.6 (4)
C7—C2—C3	118.9 (3)	N2—C22—H22	118.7
C7—C2—C1	119.8 (4)	C21—C22—H22	118.7
C3—C2—C1	121.1 (4)	N2—C23—C24	123.0 (3)
C4—C3—C2	120.0 (4)	N2—C23—H23	118.5
C4—C3—H3	120.0	C24—C23—H23	118.5
C2—C3—H3	120.0	C23—C24—C20	119.6 (4)
C3—C4—C5	121.4 (4)	C23—C24—H24	120.2
C3—C4—H4	119.3	C20—C24—H24	120.2
C5—C4—H4	119.3	N3—C25—H25A	109.5
C6—C5—C4	118.3 (3)	N3—C25—H25B	109.5
C6—C5—C8	122.2 (3)	H25A—C25—H25B	109.5
C4—C5—C8	119.5 (3)	N3—C25—H25C	109.5
C5—C6—C7	120.8 (4)	H25A—C25—H25C	109.5
C5—C6—H6	119.6	H25B—C25—H25C	109.5
C7—C6—H6	119.6	N3—C26—H26A	109.5
C2—C7—C6	120.6 (4)	N3—C26—H26B	109.5
C2—C7—H7	119.7	H26A—C26—H26B	109.5
C6—C7—H7	119.7	N3—C26—H26C	109.5
N1—C8—C9	122.8 (3)	H26A—C26—H26C	109.5
N1—C8—C5	115.0 (3)	H26B—C26—H26C	109.5
C9—C8—C5	122.2 (3)	O5—C27—N3	124.9 (5)
C10—C9—C8	119.2 (3)	O5—C27—H27	117.6
C10—C9—H9	120.4	N3—C27—H27	117.6
C8—C9—H9	120.4	N4—C28—H28A	109.5

C9—C10—C11	117.7 (3)	N4—C28—H28B	109.5
C9—C10—C20	122.1 (3)	H28A—C28—H28B	109.5
C11—C10—C20	120.2 (3)	N4—C28—H28C	109.5
C12—C11—C10	119.9 (3)	H28A—C28—H28C	109.5
C12—C11—H11	120.1	H28B—C28—H28C	109.5
C10—C11—H11	120.1	N4—C29—H29A	109.5
N1—C12—C11	122.3 (3)	N4—C29—H29B	109.5
N1—C12—C13	115.9 (3)	H29A—C29—H29B	109.5
C11—C12—C13	121.8 (3)	N4—C29—H29C	109.5
C14—C13—C18	118.8 (3)	H29A—C29—H29C	109.5
C14—C13—C12	119.9 (3)	H29B—C29—H29C	109.5
C18—C13—C12	121.3 (3)	O6—C30—N4	128.2 (7)
C15—C14—C13	120.9 (4)	O6—C30—H30	115.9
C15—C14—H14	119.6	N4—C30—H30	115.9
C13—C14—H14	119.6	C8—N1—C12	118.2 (3)
C14—C15—C16	120.3 (4)	C23—N2—C22	117.3 (3)
C14—C15—H15	119.9	C23—N2—Cu1	121.6 (2)
C16—C15—H15	119.9	C22—N2—Cu1	120.9 (3)
C17—C16—C15	119.2 (4)	C27—N3—C25	121.1 (5)
C17—C16—C19	120.7 (4)	C27—N3—C26	121.6 (4)
C15—C16—C19	120.1 (3)	C25—N3—C26	117.3 (4)
C16—C17—C18	120.2 (4)	C30—N4—C29	125.9 (7)
C16—C17—H17	119.9	C30—N4—C28	120.2 (7)
C18—C17—H17	119.9	C29—N4—C28	113.8 (7)
C17—C18—C13	120.6 (4)	C19—O1—Cu1^{iv}	128.1 (3)
C17—C18—H18	119.7	C1—O4—H4A	109.5
C13—C18—H18	119.7	H1A—O1W—H1B	107.4
O2—C19—O1	125.4 (4)		

O3—C1—C2—C7	−8.6 (7)	C19—C16—C17—C18	179.6 (4)
O4—C1—C2—C7	173.1 (4)	C16—C17—C18—C13	−1.0 (6)
O3—C1—C2—C3	166.8 (4)	C14—C13—C18—C17	2.5 (6)
O4—C1—C2—C3	−11.4 (6)	C12—C13—C18—C17	−178.2 (3)
C7—C2—C3—C4	1.3 (6)	C17—C16—C19—O2	−167.7 (4)
C1—C2—C3—C4	−174.2 (4)	C15—C16—C19—O2	12.3 (5)
C2—C3—C4—C5	−1.1 (6)	C17—C16—C19—O1	11.0 (5)
C3—C4—C5—C6	0.6 (6)	C15—C16—C19—O1	−168.9 (4)
C3—C4—C5—C8	178.0 (4)	C9—C10—C20—C21	30.9 (6)
C4—C5—C6—C7	−0.2 (6)	C11—C10—C20—C21	−146.3 (4)
C8—C5—C6—C7	−177.6 (4)	C9—C10—C20—C24	−153.5 (4)
C3—C2—C7—C6	−1.0 (6)	C11—C10—C20—C24	29.2 (5)
C1—C2—C7—C6	174.6 (4)	C24—C20—C21—C22	−3.5 (6)
C5—C6—C7—C2	0.5 (6)	C10—C20—C21—C22	172.2 (4)
C6—C5—C8—N1	167.3 (3)	C20—C21—C22—N2	0.6 (6)
C4—C5—C8—N1	−10.0 (5)	N2—C23—C24—C20	0.7 (6)
C6—C5—C8—C9	−11.9 (6)	C21—C20—C24—C23	2.9 (6)
C4—C5—C8—C9	170.7 (4)	C10—C20—C24—C23	−172.8 (4)
N1—C8—C9—C10	−1.8 (6)	C9—C8—N1—C12	1.4 (5)

C5—C8—C9—C10	177.3 (3)	C5—C8—N1—C12	−177.9 (3)
C8—C9—C10—C11	1.2 (5)	C11—C12—N1—C8	−0.4 (5)
C8—C9—C10—C20	−176.1 (3)	C13—C12—N1—C8	−179.9 (3)
C9—C10—C11—C12	−0.3 (5)	C24—C23—N2—C22	−3.6 (6)
C20—C10—C11—C12	177.1 (3)	C24—C23—N2—Cu1	171.8 (3)
C10—C11—C12—N1	−0.1 (6)	C21—C22—N2—C23	3.0 (6)
C10—C11—C12—C13	179.4 (3)	C21—C22—N2—Cu1	−172.4 (3)
N1—C12—C13—C14	28.6 (5)	O1^{i}—Cu1—N2—C23	−34.5 (3)
C11—C12—C13—C14	−151.0 (4)	O1^{ii}—Cu1—N2—C23	145.5 (3)
N1—C12—C13—C18	−150.7 (4)	O1^{i}—Cu1—N2—C22	140.8 (3)
C11—C12—C13—C18	29.8 (6)	O1^{ii}—Cu1—N2—C22	−39.2 (3)
C18—C13—C14—C15	−2.7 (6)	O5—C27—N3—C25	179.0 (5)
C12—C13—C14—C15	178.1 (4)	O5—C27—N3—C26	2.5 (8)
C13—C14—C15—C16	1.3 (6)	O6—C30—N4—C29	171.2 (8)
C14—C15—C16—C17	0.3 (6)	O6—C30—N4—C28	−10.0 (14)
C14—C15—C16—C19	−179.8 (4)	O2—C19—O1—Cu1^{iv}	−6.5 (6)
C15—C16—C17—C18	−0.4 (6)	C16—C19—O1—Cu1^{iv}	174.9 (2)

Symmetry codes: (i) −*x*+3/2, *y*−1/2, −*z*+1/2; (ii) *x*+1/2, −*y*+3/2, *z*−1/2; (iii) −*x*+2, −*y*+1, −*z*; (iv) −*x*+3/2, *y*+1/2, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4*A*···O2^{v}	0.82	1.86	2.584 (4)	146
O1*W*—H1*A*···O5^{vi}	0.85	1.98	2.808 (5)	165
O1*W*—H1*B*···O2^{i}	0.85	1.95	2.758 (4)	159

Symmetry codes: (i) −*x*+3/2, *y*−1/2, −*z*+1/2; (v) *x*+1/2, −*y*+5/2, *z*−1/2; (vi) *x*+1, *y*, *z*.