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catena-Poly[[[(2,2′-bipyridylamine-κ^2N,N')copper(II)]-μ_2-L-aspartate-$\kappa^3O,N:O'$] monohydrate]

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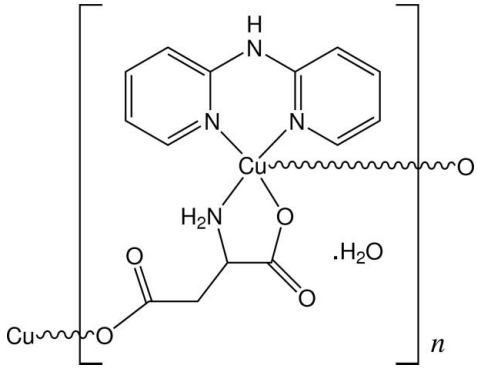
Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.006 Å; R factor = 0.040; wR factor = 0.079; data-to-parameter ratio = 15.5.

In the title complex, $\{[Cu(C_4H_5O_4N)(C_{10}H_9N_3)]\cdot H_2O\}_n$, the Cu atom has a distorted CuO_2N_3 square-pyramidal geometry formed by an *N*,*O*-bidentate aspartate (asp) anion and an *N*,*N*-bidentate 2,2′-bipyridylamine (bpa) molecule in the basal positions, and an *O*-monodentate asp ligand in the apical site. The complex forms a polymeric chain in which each metal centre is bridged to the next one by the asp anion. The crystal structure is stabilized by O—H···O and N—H···O hydrogen bonds and π–π stacking interactions involving the bpa ligands [centroid–centroid separation = 3.699 (4) Å].

Related literature

For related structures, see: Antolini *et al.* (1983, 1985). For background, see: Kelland (2005); Wang & Okabe (2005); Yodoshi *et al.* (2007).



Experimental

Crystal data

$[Cu(C_4H_5O_4N)(C_{10}H_9N_3)]\cdot H_2O$
M_r = 383.86
Orthorhombic, $P2_12_12_1$
a = 7.018 (5) Å
b = 10.364 (8) Å
c = 20.72 (2) Å
V = 1507 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.48 mm^{-1}
T = 123.1 K
0.40 × 0.04 × 0.04 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.931, T_{max} = 0.942
13783 measured reflections
3469 independent reflections
2022 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.061

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.079
S = 0.94
3469 reflections
224 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.85 e Å^{-3}
$\Delta\rho_{min}$ = −0.90 e Å^{-3}
Absolute structure: Flack (1983), with 1416 Friedel pairs
Flack parameter: 0.02 (2)

Table 1
Selected bond lengths (Å).

Cu1—O1	1.958 (2)	Cu1—N2	1.981 (3)
Cu1—O3^{i}	2.157 (2)	Cu1—N4	2.015 (3)
Cu1—N1	1.997 (3)		

Symmetry code: (i) $x+1, y, z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H9···O4^{ii}	0.86	1.97	2.763 (4)	153
N4—H10···O5	0.90	2.15	3.031 (4)	166
N4—H11···O4	0.90	2.19	2.793 (4)	124
O5—H15···O3^{iii}	0.82	2.08	2.867 (3)	160
O5—H16···O2^{iii}	0.84	1.92	2.756 (4)	173

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2005) and *CRYSTALS* (Betteridge *et al.*, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *CrystalStructure*.

The authors thank Kinki University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2533).

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supplementary materials

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catena-Poly[[[(2,2'-bipyridylamine-κ^2N,N')copper(II)]-μ_2-L-aspartate-$\kappa^3O,N:O'$] monohydrate]

N. Okabe, M. Mototsuji and M. Yodoshi

Comment

Recently, significant attention has focused on Cu(II) complexes in the studies of their antitumor and/or antiviral activity (Wang & Okabe, 2005; Kelland, 2005).

As part of our ongoing studies (Yodoshi *et al.*, 2007) of mixed-ligand copper complexes, we now report the synthesis and structure of the title compound, (I), containing both aspartate (asp) anions and 2,2'-bipyridylamine (bpa) molecules (Fig. 1).

The Cu atom in (I) has a distorted square-pyramidal geometry formed by one O atom of the α-carboxylate group, one N atom of the α-amino group of an aspartate anion and two N atoms of a bidentate bpa in the basal plane and one O atom from the β-carboxylate of an aspartate in the axial position. Each complex is bridged through the O atom in the axial position, and forms polymeric chains.

Cu1 deviates by 0.289 (1) Å from the mean plane through atoms N1, N2, N4 and O1. A six-membered chelate ring Cu1/N1/C5/N3/C6/N2 and a five- membered one Cu1/O1/C11/C12/N4 are formed between the Cu1 atom and the bpa and asp ligands, respectively, where the dihedral angle between two planes, Cu1/N1/N2 and Cu1/O1/N4 is 23.1 (2)°. The two pyridine rings in the bpa ligand are also non-planar with the dihedral angle of 23.15 (8)°.

The metal coordination in (I) resembles that in monomeric Cu(asp)(bpy)H_2O (Antolini *et al.*, 1983), and the polymeric linear chain structure of (I) resembles that in $[Cu(glu)(bpy)]_n$ (Antolini *et al.*, 1985).

The bond distances (Table 1) in the square plane in (I) are similar to those in Cu(asp)(bpy)H_2O and $[Cu(glu)(bpy)]_n$. The Cu1—O3 bond lenght is a little longer than those in the square plane because of the well known Jahn-Teller effect. The axial distance is similar to that in the polymeric complex, $\{Cu(glu)(bpy)]_n$, but a little shorter than that in Cu(asp)(bpy)H_2O.

The crystal structure of (I) is stabilized by O—H···O hydrogen bonds the water molecules and the carboxylate group of asp, and N—H···O hydrogen bonds between the imino group of bpa and the carboxylate group (Table 2). Aromatic π-π stacking interactions between bpa ligands of adjacent chains also stabilizes the crystal packing (Fig. 2). The distance between the centroids of the pyridine rings *Cg*1 (N1/C1—C5) and *Cg*2 (N2/C6—C10) (symmetry code: −1/2 + *x*, 1/2 − *y*, 1 − *z*) is 3.699 (4) Å (Spek, 2003).

Experimental

Bpa (50.0 mg) was mixed with $CuCl_2{\cdot}2H_2O$ (49.8 mg), in 5 ml of 80% (*v*/*v*) methanol-water solution for 5 min at room temperature (molar ratio 1:1). The aquamarine-colored precipitate was dried under a vacuum and assumed to be $[Cu(bpa)Cl_2]$. Then, the precipitate (5.0 mg) was reacted with aspartic acid (2.0 mg) in 2.4 ml dimethylsulfoxide for 60 min at 343 K. The reaction mixture was left to stand at room temperature, and after two months, blue needles of (I) appeared from the mother liquor.

Refinement

The water H atoms were located in a difference map and refined as riding in their as-found relative positions with U_{iso}(H) = 1.5U_{eq}(O).

The other H atoms were located in a difference map, relocated in idealized locations (C—H = 0.93–0.97 Å, N—H = 0.86 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C, N)

Figures

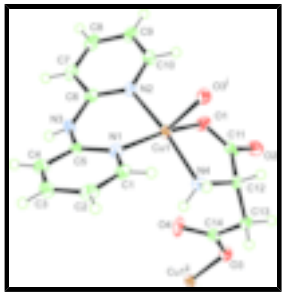

Fig. 1. The asymmetric unit of (I) expanded to show the polymeric connectivity with displacement ellipsoids shown at the 50% probability level (arbitrary spheres for the H atoms). The uncoordinated water molecule is omitted for clarity. Symmetry codes: (i) 1 + *x*, *y*, *z*; (ii) −1 + *x*, *y*, *z*.

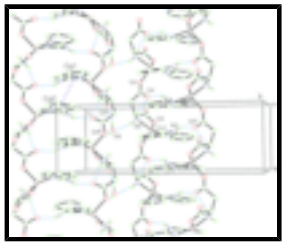

Fig. 2. A view of the hydrogen bonding (blue dashed lines) and π-π stacking (purple dashed lines) interactions in (I). See the text for the designations of *Cg*1 and *Cg*2 [at (−1/2 + *x*, 1/2 − *y*, 1 − *z*)]. Symmetry codes: (i) *x* + 1/2, −*y* + 1/2, −*z* + 1; (ii) −*x*, *y* + 1/2, −*z* + 3/2.

catena-Poly[[[(2,2'-bipyridylamine-κ^2*N*,*N*')copper(II)]- μ$_2$-*L*-aspartate-κ^3*O*,*N*:*O*'] monohydrate]

Crystal data

$[Cu(C_4H_5O_4N)(C_{10}H_9N_3)]\cdot H_2O$	F_{000} = 788.00
M_r = 383.86	D_x = 1.692 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.7107 Å
Hall symbol: P 2ac 2ab	Cell parameters from 11236 reflections
a = 7.018 (5) Å	θ = 3.1–27.5º
b = 10.364 (8) Å	μ = 1.48 mm^{-1}
c = 20.72 (2) Å	*T* = 123.1 K
V = 1507 (2) Å^3	Needle, blue
Z = 4	0.40 × 0.04 × 0.04 mm

Data collection

Rigaku R-AXIS RAPID diffractometer	2022 reflections with $F^2 > 2.0\sigma(F^2)$

Detector resolution: 10.00 pixels mm^{-1}

ω scans

Absorption correction: multi-scan (ABSCOR; Higashi, 1995)

T_{min} = 0.931, T_{max} = 0.942

13783 measured reflections

3469 independent reflections

R_{int} = 0.061

θ_{max} = 27.5º

h = −9→8

k = −13→13

l = −26→26

Refinement

Refinement on F^2

$R[F^2 > 2\sigma(F^2)]$ = 0.040

$wR(F^2)$ = 0.079

S = 0.94

3469 reflections

224 parameters

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0362P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max}$ = 0.85 e $Å^{-3}$

$\Delta\rho_{min}$ = −0.90 e $Å^{-3}$

Extinction correction: none

Absolute structure: Flack (1983), 1416 Friedel pairs

Flack parameter: 0.02 (2)

Special details

Geometry. ENTER SPECIAL DETAILS OF THE MOLECULAR GEOMETRY

Refinement. Refinement using all reflections. The weighted *R*-factor (*wR*) and goodness of fit (*S*) are based on F^2. *R*-factor (gt) are based on *F*. The threshold expression of $F^2 > 2.0\ \sigma(F^2)$ is used only for calculating *R*-factor (gt).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.36399 (6)	0.09559 (4)	0.61800 (2)	0.0172 (1)
O1	0.2334 (3)	−0.0709 (2)	0.6236 (1)	0.0242 (6)
O2	0.0185 (4)	−0.1830 (3)	0.6789 (1)	0.0292 (7)
O3	−0.4093 (3)	0.0429 (2)	0.6832 (1)	0.0209 (6)
O4	−0.1666 (4)	0.1431 (3)	0.6343 (1)	0.0297 (7)
O5	0.3663 (4)	0.2681 (2)	0.8106 (1)	0.0279 (6)
N1	0.4276 (4)	0.2784 (3)	0.5966 (1)	0.0168 (7)
N2	0.4572 (4)	0.0421 (3)	0.5318 (1)	0.0178 (7)
N3	0.3895 (4)	0.2443 (3)	0.4851 (1)	0.0197 (7)
N4	0.1925 (4)	0.1424 (3)	0.6924 (1)	0.0177 (7)
C1	0.4647 (5)	0.3616 (4)	0.6454 (2)	0.0209 (9)
C2	0.4876 (5)	0.4911 (4)	0.6369 (2)	0.025 (1)
C3	0.4779 (5)	0.5399 (4)	0.5744 (2)	0.0248 (9)
C4	0.4460 (5)	0.4572 (4)	0.5240 (2)	0.0250 (9)
C5	0.4214 (5)	0.3259 (3)	0.5365 (2)	0.0162 (8)
C6	0.4331 (5)	0.1137 (4)	0.4789 (2)	0.0193 (8)
C7	0.4491 (5)	0.0626 (4)	0.4165 (2)	0.0230 (9)
C8	0.4944 (5)	−0.0649 (4)	0.4100 (2)	0.0271 (9)
C9	0.5273 (5)	−0.1404 (4)	0.4643 (2)	0.0250 (9)

C10	0.5064 (5)	−0.0835 (4)	0.5240 (2)	0.0235 (8)
C11	0.1157 (5)	−0.0845 (3)	0.6693 (2)	0.0213 (8)
C12	0.0989 (5)	0.0253 (3)	0.7183 (2)	0.0174 (8)
C13	−0.1098 (5)	0.0490 (3)	0.7371 (2)	0.0178 (8)
C14	−0.2371 (5)	0.0801 (4)	0.6797 (2)	0.0189 (8)
H1	0.4750	0.3286	0.6870	0.025*
H2	0.5091	0.5454	0.6719	0.030*
H3	0.4930	0.6278	0.5670	0.030*
H4	0.4407	0.4882	0.4819	0.030*
H5	0.4294	0.1143	0.3804	0.028*
H6	0.5034	−0.1013	0.3691	0.033*
H7	0.5622	−0.2266	0.4605	0.030*
H8	0.5271	−0.1335	0.5605	0.028*
H9	0.3351	0.2789	0.4522	0.024*
H10	0.2615	0.1804	0.7237	0.021*
H11	0.1034	0.1988	0.6790	0.021*
H12	0.1678	−0.0007	0.7574	0.021*
H13	−0.1588	−0.0272	0.7586	0.021*
H14	−0.1153	0.1200	0.7675	0.021*
H15	0.4061	0.3424	0.8139	0.042*
H16	0.2480	0.2763	0.8131	0.042*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0183 (2)	0.0164 (2)	0.0169 (2)	−0.0009 (2)	0.0007 (2)	0.0000 (2)
O1	0.024 (1)	0.021 (1)	0.028 (2)	−0.005 (1)	0.010 (1)	−0.002 (1)
O2	0.029 (2)	0.017 (1)	0.042 (2)	−0.002 (1)	0.009 (1)	0.001 (1)
O3	0.017 (1)	0.024 (1)	0.022 (1)	−0.002 (1)	−0.001 (1)	0.004 (1)
O4	0.023 (1)	0.046 (2)	0.021 (2)	−0.006 (1)	0.000 (1)	0.018 (1)
O5	0.027 (1)	0.019 (1)	0.038 (2)	0.002 (2)	−0.002 (2)	−0.005 (1)
N1	0.015 (1)	0.018 (2)	0.018 (2)	−0.002 (1)	−0.001 (1)	−0.001 (1)
N2	0.021 (2)	0.018 (2)	0.014 (2)	−0.003 (1)	0.000 (1)	0.002 (1)
N3	0.023 (2)	0.020 (2)	0.015 (2)	0.001 (2)	−0.005 (1)	0.004 (1)
N4	0.015 (1)	0.017 (2)	0.021 (2)	−0.002 (1)	−0.001 (1)	−0.003 (1)
C1	0.017 (2)	0.025 (2)	0.020 (2)	−0.002 (2)	0.001 (2)	−0.002 (2)
C2	0.019 (2)	0.022 (2)	0.033 (3)	−0.006 (2)	0.002 (2)	−0.010 (2)
C3	0.027 (2)	0.017 (2)	0.030 (2)	−0.001 (2)	0.002 (2)	0.003 (2)
C4	0.020 (2)	0.024 (2)	0.031 (2)	0.003 (2)	0.005 (2)	0.004 (2)
C5	0.014 (2)	0.018 (2)	0.017 (2)	0.004 (2)	0.000 (2)	0.000 (2)
C6	0.014 (2)	0.023 (2)	0.020 (2)	−0.004 (2)	0.001 (1)	−0.002 (2)
C7	0.025 (2)	0.026 (2)	0.018 (2)	−0.007 (2)	0.001 (2)	0.000 (2)
C8	0.031 (2)	0.032 (3)	0.018 (2)	−0.006 (2)	0.004 (2)	−0.006 (2)
C9	0.032 (2)	0.020 (2)	0.023 (2)	−0.004 (2)	0.009 (2)	−0.004 (2)
C10	0.025 (2)	0.021 (2)	0.025 (2)	−0.001 (2)	0.004 (2)	0.005 (2)
C11	0.018 (2)	0.012 (2)	0.034 (2)	−0.002 (2)	−0.005 (2)	0.005 (2)
C12	0.017 (2)	0.018 (2)	0.017 (2)	−0.002 (2)	−0.001 (2)	0.004 (1)
C13	0.018 (2)	0.019 (2)	0.016 (2)	−0.003 (2)	0.001 (2)	−0.001 (1)

C14	0.016 (2)	0.019 (2)	0.022 (2)	0.002 (2)	−0.002 (1)	−0.003 (2)

Geometric parameters (Å, °)

Cu1—O1	1.958 (2)	C2—C3	1.391 (6)
Cu1—O3^{i}	2.157 (2)	C2—H2	0.9300
Cu1—N1	1.997 (3)	C3—C4	1.370 (6)
Cu1—N2	1.981 (3)	C3—H3	0.9300
Cu1—N4	2.015 (3)	C4—C5	1.396 (5)
O1—C11	1.264 (4)	C4—H4	0.9302
O2—C11	1.245 (4)	C6—C7	1.402 (5)
O3—Cu1^{ii}	2.157 (2)	C7—C8	1.366 (6)
O3—C14	1.271 (4)	C7—H5	0.9300
O4—C14	1.247 (4)	C8—C9	1.390 (5)
O5—H15	0.8220	C8—H6	0.9300
O5—H16	0.8365	C9—C10	1.377 (5)
N1—C1	1.354 (5)	C9—H7	0.9301
N1—C5	1.340 (5)	C10—H8	0.9300
N2—C6	1.335 (5)	C11—O1	1.264 (4)
N2—C10	1.357 (5)	C11—O2	1.245 (4)
N3—C5	1.378 (5)	C11—C12	1.530 (5)
N3—C6	1.394 (5)	C12—C11	1.530 (5)
N3—H9	0.8599	C12—C13	1.535 (5)
N4—C12	1.482 (4)	C12—H12	0.9800
N4—H10	0.9001	C13—C14	1.522 (5)
N4—H11	0.9000	C13—H13	0.9700
C1—C2	1.363 (5)	C13—H14	0.9700
C1—H1	0.9300	H16—O5	0.8365
O1—Cu1—O3^{i}	94.9 (1)	C4—C3—C2	119.3 (4)
O1—Cu1—N1	162.7 (1)	C4—C3—H3	120.3422
O1—Cu1—N2	87.8 (1)	H3—C3—C2	120.3249
O1—Cu1—N4	83.5 (1)	C5—C4—C3	119.3 (4)
O3^{i}—Cu1—N1	102.4 (1)	C5—C4—H4	120.3693
O3^{i}—Cu1—N2	104.5 (1)	H4—C4—C3	120.3705
O3^{i}—Cu1—N4	91.3 (1)	C7—C6—N2	122.5 (3)
N1—Cu1—N2	89.5 (1)	C7—C6—N3	118.0 (3)
N1—Cu1—N4	94.3 (1)	C8—C7—C6	118.3 (3)
N2—Cu1—N4	162.6 (1)	C8—C7—H5	120.8306
C11—O1—Cu1	116.6 (2)	H5—C7—C6	120.8366
Cu1^{ii}—O3—C14	126.1 (2)	C9—C8—C7	120.3 (4)
H15—O5—H16	103.7063	C9—C8—H6	119.8735
C1—N1—Cu1	118.8 (2)	H6—C8—C7	119.8668
C1—N1—C5	117.8 (3)	C10—C9—C8	117.9 (4)
C5—N1—Cu1	123.2 (2)	C10—C9—H7	121.0512
C6—N2—Cu1	122.9 (2)	H7—C9—C8	121.0527
C6—N2—C10	117.8 (3)	H8—C10—N2	118.4655
C10—N2—Cu1	117.4 (2)	H8—C10—C9	118.4670

C5—N3—C6	129.2 (3)	O1—C11—C12	117.7 (3)
C5—N3—H9	115.4117	O1—C11—O2	124.7 (3)
C6—N3—H9	115.4095	O2—C11—C12	117.5 (3)
C12—N4—Cu1	110.2 (2)	C11—C12—N4	109.5 (3)
C12—N4—H10	109.6151	C11—C12—H12	107.8129
C12—N4—H11	109.6255	C11—C12—C13	111.1 (3)
H10—N4—Cu1	109.6205	C13—C12—N4	112.5 (3)
H10—N4—H11	108.1428	C13—C12—H12	107.8132
H11—N4—Cu1	109.6256	H12—C12—N4	107.8176
C2—C1—N1	123.5 (4)	C14—C13—C12	113.3 (3)
C2—C1—H1	118.2291	C14—C13—H13	108.8942
H1—C1—N1	118.2395	C14—C13—H14	108.9045
C3—C2—C1	118.2 (4)	H13—C13—C12	108.9037
C3—C2—H2	120.8867	H13—C13—H14	107.7389
H2—C2—C1	120.8839	H14—C13—C12	108.9029
N1—Cu1—O1—C11	−87.8 (4)	N1—C1—C2—C3	−1.9 (6)
O1—Cu1—N1—C1	124.4 (3)	C1—C2—C3—C4	0.0 (5)
O1—Cu1—N2—C6	126.6 (3)	C2—C3—C4—C5	0.8 (5)
O1—Cu1—N4—C12	11.8 (2)	C3—C4—C5—N1	0.2 (4)
Cu1—O1—C11—O2	178.5 (3)	C3—C4—C5—N3	−179.9 (2)
Cu1—N1—C1—C2	−172.1 (3)	N2—C6—C7—C8	−1.1 (5)
Cu1—N1—C5—N3	−7.1 (4)	C6—C7—C8—C9	−1.3 (5)
Cu1—N1—C5—C4	172.7 (3)	C7—C8—C9—C10	2.1 (6)
Cu1—N2—C6—N3	18.2 (4)	C8—C9—C10—N2	−0.5 (6)
Cu1—N2—C10—C9	163.3 (3)	O1—C11—C12—N4	14.4 (4)
C6—N3—C5—N1	−28.1 (5)	O2—C11—C12—N4	−168.6 (3)
C6—N3—C5—C4	152.1 (3)	N4—C12—C13—C14	65.7 (4)
C5—N3—C6—N2	22.1 (5)	C12—C13—C14—O3	147.9 (3)
Cu1—N4—C12—C11	−16.4 (3)	C12—C13—C14—O4	−34.3 (5)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H9···O4^{iii}	0.86	1.97	2.763 (4)	153
N4—H10···O5	0.90	2.15	3.031 (4)	166
N4—H11···O4	0.90	2.19	2.793 (4)	124
O5—H15···O3^{iv}	0.82	2.08	2.867 (3)	160
O5—H16···O2^{iv}	0.84	1.92	2.756 (4)	173

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

Fig. 1

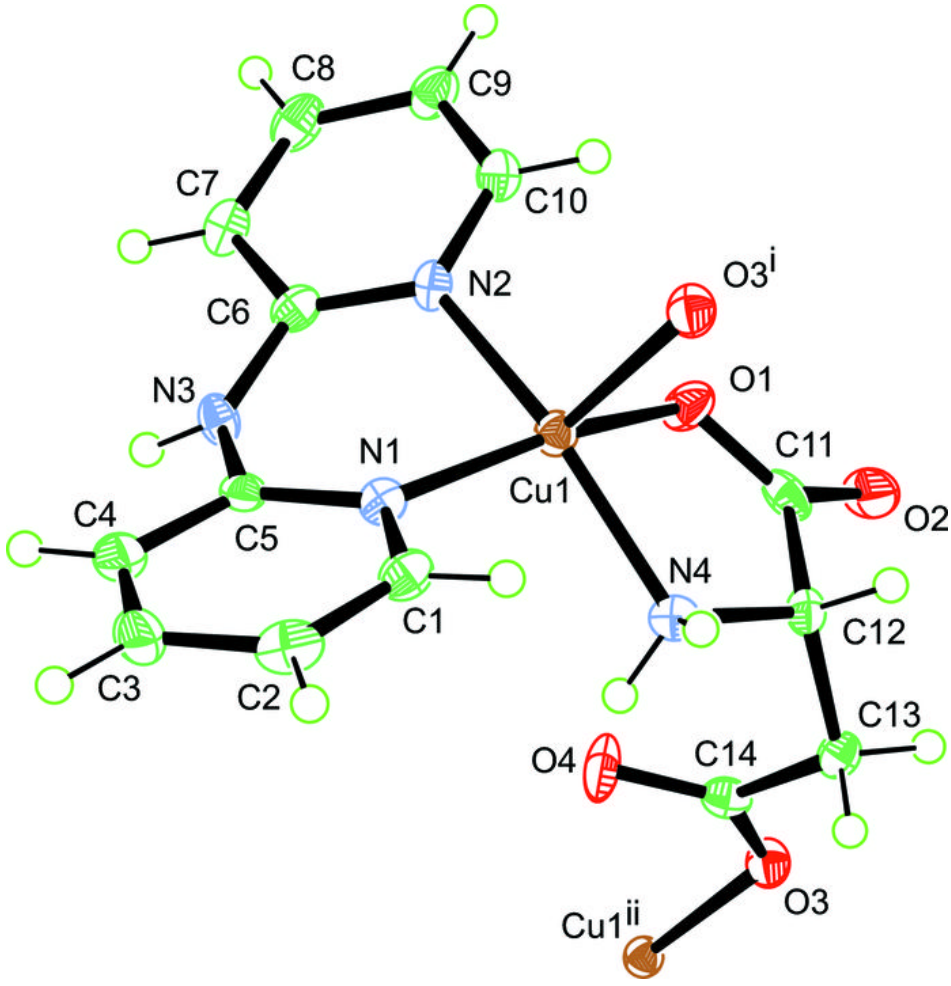
C8
C9
C7
C10
N2
O3i
C6
O1
N3
C11
N1
Cu1
O2
C4
C5
N4
C1
C12
C3
C2
C13
O4
C14
O3
Cu1ii

Fig. 2