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trans-Diaquabis(ethylenediamine-κ^2N,N')copper(II) bis[3-(3-pyridyl)-propionate] dihydrate

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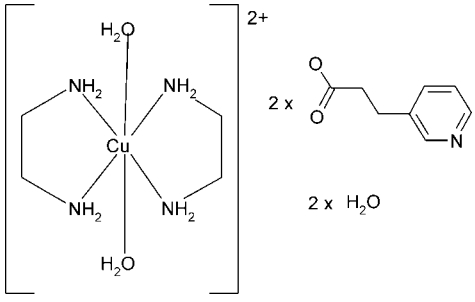
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.004 Å; R factor = 0.042; wR factor = 0.087; data-to-parameter ratio = 18.7.

The asymmetric unit of the title complex, $[Cu(C_2H_8N_2)_2(H_2O)_2](C_8H_8NO_2)_2\cdot 2H_2O$, contains one anion, one half-cation and one water molecule. The Cu^{II} atom in the $[Cu(en)_2(H_2O)_2]^{2+}$ cation (en is ethylenediamine) lies on an inversion centre. The four N atoms of the en ligands in the equatorial plane around the Cu^{II} atom form a slightly distorted square-planar arrangement, while the slightly distorted Jahn–Teller octahedral coordination is completed by two water O atoms in axial positions. In the crystal structure, intra- and intermolecular N—H···O and O—H···O hydrogen bonds form a three-dimensional network.

Related literature

For general background, see: Hathaway & Hodgson (1973); Bernstein *et al.* (1995); Janiak (2000); Jeffrey (1997). For similar structures, see: Jašková *et al.* (2007); Miminoshvili *et al.* (2005); Carballo *et al.* (2005); Segla *et al.* (2000); Liu *et al.* (2004); Sharma *et al.* (2005); Anacona *et al.* (2002); Emsley *et al.* (1988, 1990); Li *et al.* (2005); Gonzalez-Alvarez *et al.* (2003); Lee *et al.* (2005); Mahadevan *et al.* (1986); Kovbasyuk *et al.* (1997); Harrison *et al.* (2007).



Experimental

Crystal data

$[Cu(C_2H_8N_2)_2(H_2O)_2](C_8H_8NO_2)_2\cdot 2H_2O$
M_r = 556.13
Triclinic, $P\overline{1}$
a = 6.2620 (1) Å
b = 8.5660 (2) Å
c = 13.3550 (4) Å
α = 75.271 (1)°
β = 83.809 (1)°
γ = 70.863 (1)°
V = 654.30 (3) Å^3
Z = 1
Ag $K\alpha$ radiation
μ = 0.47 mm^{-1}
T = 153 (2) K
0.45 × 0.25 × 0.20 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Absorption correction: numerical (*HABITUS*; Herrendorf & Bärnighausen, 1997)
T_{min} = 0.808, T_{max} = 0.915
15039 measured reflections
2989 independent reflections
2644 reflections with $I > 2\sigma(I)$
R_{int} = 0.079

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.086
S = 1.07
2989 reflections
160 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O2^{i}	0.92	2.32	3.130 (3)	147
N1—H1A···O1^{i}	0.92	2.41	3.247 (2)	152
N1—H1B···O2W	0.92	2.11	2.944 (3)	151
N2—H2A···O1^{ii}	0.92	2.29	3.150 (3)	155
N2—H2B···O1	0.92	2.12	3.019 (2)	164
O1W—H1W···O2^{i}	0.84	2.06	2.873 (3)	164
O1W—H2W···O1	0.84	2.00	2.814 (2)	164
O2W—H3W···N3^{iii}	0.84	2.08	2.899 (3)	163
O2W—H4W···O2^{iv}	0.84	2.03	2.859 (3)	169

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

Data collection: *KappaCCD Software* (Nonius, 1997); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2427).

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Acta Cryst. (2008). E**64**, m509–m510 [doi:10.1107/S1600536808005400]

trans-Diaquabis(ethylenediamine-κ^2N,N')copper(II) bis[3-(3-pyridyl)propionate] dihydrate

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S1. Comment

It is well known that copper(II) complexes having ethylenediamine (en) ligands show flexible coordination environment and adopt semi-coordation with tetragonal distortion. As part of our efforts to investigate metal(II) complexes based on pyridyl-carboxylic acids, we report herein the crystal structure of the title compound, (I).

The asymmetric unit of (I), (Fig. 1), contains one anion, one half-cation and one water molecule. The Cu^{II} atom in the centrosymmetric $[Cu(en)_2(H_2O)_2]^{2+}$ cation lies on the inversion centre. The four N atoms of the ethylenediamine ligands in the equatorial plane around the Cu^{II} atom form a slightly distorted square-planar arrangement, while the slightly distorted Jahn-Teller octahedral coordination is completed by the two O atoms of water molecules in the axial positions (Table 1 and Fig. 1).

The Cu—N1 [2.015 (2) Å] and Cu—N2 [2.022 (2) Å] bond lengths and N1—Cu—N2 [84.91 (7)°] bond angle agree with those found in other $[Cu(en)_2(H_2O)_2]^{2+}$ complexes (Table 1). The Cu—O1W [2.503 (2) Å] bond is much longer than Cu—N bonds, as a result of the Jahn-Teller distortion. The Cu—OW bonds in other $[Cu(en)_2(H_2O)_2]^{2+}$ complexes are in the range of 2.416 (3)–2.693 (9) Å (Table 1). The value of the T parameter (Hathaway & Hodgson, 1973), which indicates the degree of tetragonal distortion about the Cu^{II} atom, is 0.81 and it agrees with the reported values, in the range of 0.76–0.84, for other $[Cu(en)_2(H_2O)_2]^{2+}$ complexes (Table 1).

In the crystal structure, the $[Cu(en)_2(H_2O)_2]^{2+}$ coordination cations and 3-(3-pyridyl)propionate anions are linked by O—H···O and N—H···O hydrogen-bonds (Table 2, Fig. 2) in parallel to the *a* axis. The amine H atom is linked to both carboxylate O atoms of 3-(3-pyridyl)propionate by three-centered/bifurcated N—H···O hydrogen-bonds (Jeffrey, 1997) and both of them form the $R_1^2(4)$ ring motif (Bernstein *et al.*, 1995). The similar $R_1^2(4)$ ring motifs with sulfonate or carboxylate groups are reported in$[Cu(en)_2(H_2O)_2]$(4-amino- naphthalene-1-sulfonate)$_2$.2 H_2O (Li *et al.*, 2005)and $[Cu(en)_2(H_2O)_2]$- (*N*-carboxyglycinate).H_2O (Kovbasyuk *et al.*, 1997).

The O—H···O hydrogen bonds between the coordinated water molecules and the carboxylate O atoms of 3-(3-pyridyl)-propionate anions and N—H···O hydrogen bonds of amine H atoms form the $R_2^1(6)$ and $R_2^2(8)$ ring motifs (Bernstein *et al.*, 1995). These ring motifs are also reported for other $[Cu(en)_2(H_2O)_2]X_2$ complexes, while only the $R_2^2(8)$ ring motifs are present in $[Cu(en)_2(H_2O)_2]X_2$ complexes, [where X = 4-chlorobenzoate (Lee *et al.*, 2005); X = 4-fluorobenzoate (Liu *et al.*, 2004), X = isonicotinate (Segla *et al.*, 2000) and X = 4-nitrobenzoate (Harrison *et al.*, 2007)]. On the other hand, the $R_2^1(6)$ ring motifs are reported for $[Cu(en)_2(H_2O)_2]X_2$ complexes, [where X = naphthalene-2-sulfonate (Sharma *et al.*, 2005) and X = 2,6-dimethoxynicotinate (Jašková *et al.*, 2007)]. To the best of our knowledge, only $[Cu(en)_2(H_2O)_2]$(2-aminobenzoate)$_2$ complex (Miminoshvili *et al.*, 2005), exhibits both $R_2^1(6)$ and $R_2^2(8)$ ring motifs, in the crystal structure.

The additional N—H···O hydrogen bonds form further $R_2^1(6)$ ring motifs. Finally, two $[Cu(en)_2(H_2O)_2]^{2+}$ cations and two 3-(3-pyridyl)propionate anions are joined through $R_4^2(8)$ ring motifs to form a layer parallel to the *a* axis. The layers of

$[Cu(en)_2(H_2O)_2]^{2+}$ cations and 3-(3-pyridyl)- propionate anions are linked to form a three-dimensional network through uncoordinated water molecules by O—H···O and O—H···N hydrogen-bonds (Fig. 3).

The additional interactions between the 3-(3-pyridyl)propionate anions of (I) are the π-π stacking interactions (Janiak, 2000) between the two adjacent pyridine rings, (N3/C6—C10), with the centroid to centroid distances of $C_g\cdots C_g^{v}$ = 3.66 Å [symmetry code: (v) -*x*,-*y* + 2,-*z* + 2]. The distance between parallel planes of the stacked pyridine rings is 3.33 Å.

S2. Experimental

The violet $[Cu(en)_2(H_2O)_2](3\text{-pypr})_2.2H_2O$ was formed in a methanolic solution of $[Cu(3\text{-pypr})_2(H_2O)_2]$ (1.25 mmol) by adding ethylenediamine in the molar ratio of 1:2. The resulting solution was left to slowly evaporate at room temperature. In isolating the complex, it was necessary to add acetone to the concentrated solution. Well shaped violet crystals, suitable for X-ray structure analysis were collected after a few hours by filtration and finally dried *in vacuo* (yield; 90%). Anal. Calc. for $C_{20}H_{40}N_6O_8$; C, 43.20; H, 7.25; N, 15.11; Cu, 11.43. Found: C, 43.45; H, 7.47; N, 15.30; Cu, 11.21%. Selected IR data (cm^{-1}): 1592 *versus*,br ($\nu_a(COO^-)$ + ν(C?N)); 1392 *versus* ($\nu_s(COO^-)$); 605 s (δ(py), pyridine ring in-plane bending); 405 m (γ(py), pyridine ring out-of-plane bending). Electronic data (cm^{-1}): 18 400 br.

S3. Refinement

H atoms were positioned geometrically, with O—H = 0.84 Å (for H_2O), N—H = 0.92 Å (for NH_2) and C—H = 0.95 and 0.99 Å for aromatic and methylene H, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C,*N*,*O*), where *x* = 0.92 for O2W H and *x* = 1.2 for other H atoms.

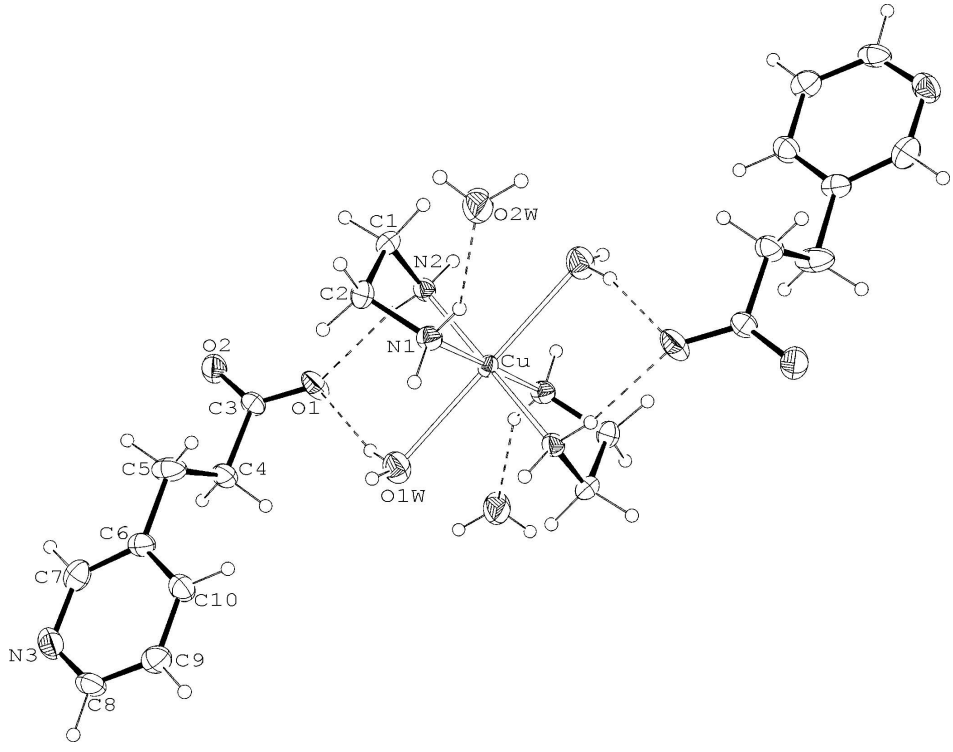

Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

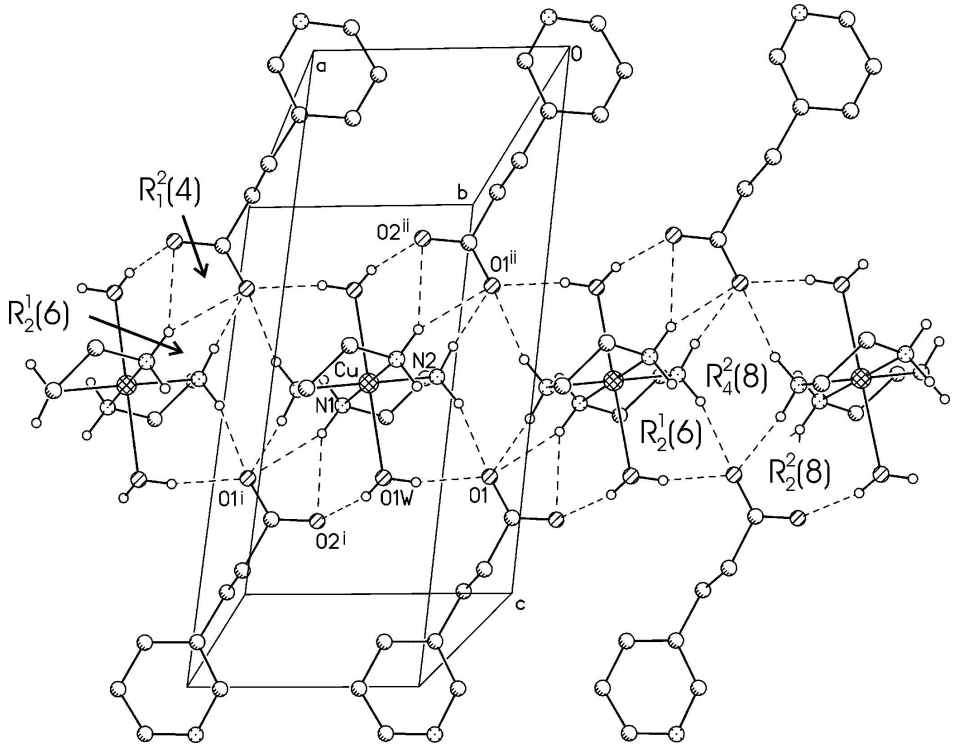

Figure 2

Part of the crystal structure of (I), showing the formation of $R^2_1(4)$, $R^1_2(6)$, $R^2_4(8)$ and $R^2_2(8)$ motifs [symmetry codes: (i) $x + 1, y, z$; (ii) $-x, -y + 1, -z + 1$].

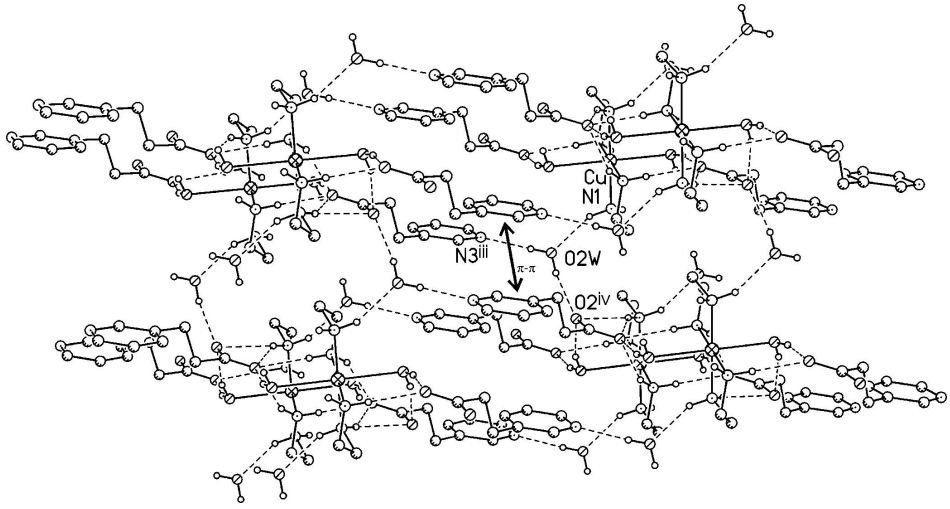

Figure 3

A packing diagram of (I), showing hydrogen bonds and π-π stacking interactions, as dashed lines [symmetry codes: (iii) $x + 1, y, z - 1$; (iv) $-x, -y + 2, -z + 1$].

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Crystal data

$[Cu(C_2H_8N_2)_2(H_2O)_2](C_8H_8NO_2)_2\cdot 2H_2O$
$M_r = 556.13$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.2620$ (1) Å
$b = 8.5660$ (2) Å
$c = 13.3550$ (4) Å
$\alpha = 75.271$ (1)°
$\beta = 83.809$ (1)°
$\gamma = 70.863$ (1)°
$V = 654.30$ (3) Å^3
$Z = 1$
$F(000) = 295$
$D_x = 1.411$ Mg m^{-3}
Ag $K\alpha$ radiation, $\lambda = 0.56085$ Å
Cell parameters from 2489 reflections
$\theta = 3.3$–$21.4°$
$\mu = 0.47$ mm^{-1}
$T = 153$ K
Prism, violet
0.45 × 0.25 × 0.20 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: numerical (*HABITUS*; Herrendorf & Bärnighausen, 1997)
$T_{min} = 0.808$, $T_{max} = 0.915$
15039 measured reflections
2989 independent reflections
2644 reflections with $I > 2\sigma(I)$
$R_{int} = 0.079$
$\theta_{max} = 21.4°$, $\theta_{min} = 3.3°$
$h = -8\rightarrow 8$
$k = -11\rightarrow 11$
$l = -17\rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.086$
$S = 1.07$
2989 reflections
160 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
$w = 1/[\sigma^2(F_o^2) + (0.0215P)^2 + 0.3896P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ 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.
Least-squares planes (*x*,*y*,*z* in crystal coordinates) and deviations from them (* indicates atom used to define plane)
2.3086 (0.0059) *x* + 8.2273 (0.0023) *y* - 0.2376 (0.0130) *z* = 6.3254 (0.0154)
* 0.0032 (0.0016) N3
* -0.0044 (0.0016) C6
* 0.0010 (0.0017) C7
* -0.0039 (0.0017) C8
* 0.0003 (0.0018) C9
* 0.0038 (0.0017) C10
3.3255 (0.0028) N3_$6
3.3331 (0.0028) C6_$6
3.3277 (0.0030) C7_$6
3.3326 (0.0031) C8_$6
3.3285 (0.0029) C9_$6
3.3249 (0.0030) C10_$6
Rms deviation of fitted atoms = 0.0032

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}
Cu	0.5000	0.5000	0.5000	0.02500 (12)
N1	0.5413 (3)	0.7274 (2)	0.48893 (14)	0.0328 (4)
H1A	0.6147	0.7242	0.5459	0.039*
H1B	0.6270	0.7540	0.4306	0.039*
N2	0.1813 (3)	0.6372 (2)	0.45504 (14)	0.0307 (4)
H2A	0.1410	0.5969	0.4047	0.037*
H2B	0.0813	0.6297	0.5104	0.037*
N3	−0.0294 (4)	0.8099 (3)	1.12361 (17)	0.0520 (6)
O1	−0.0720 (3)	0.6040 (3)	0.66095 (13)	0.0493 (5)
O2	−0.4121 (3)	0.7310 (2)	0.71927 (15)	0.0518 (5)
O1W	0.3984 (3)	0.4843 (2)	0.68797 (15)	0.0515 (5)
H1W	0.4422	0.5531	0.7088	0.063*
H2W	0.2570	0.5084	0.6916	0.063*
O2W	0.6770 (4)	0.9227 (3)	0.29173 (16)	0.0682 (6)
H3W	0.7363	0.8948	0.2368	0.063*
H4W	0.6086	1.0274	0.2809	0.063*
C1	0.1767 (4)	0.8158 (3)	0.41381 (19)	0.0399 (5)
H1C	0.0192	0.8928	0.4130	0.048*
H1D	0.2402	0.8312	0.3421	0.048*
C2	0.3163 (4)	0.8558 (3)	0.4831 (2)	0.0399 (5)
H2C	0.3294	0.9709	0.4542	0.048*
H2D	0.2442	0.8520	0.5530	0.048*
C3	−0.2033 (4)	0.6638 (3)	0.72904 (17)	0.0339 (5)

C4	−0.1063 (4)	0.6478 (3)	0.83208 (19)	0.0418 (5)
H4A	−0.2050	0.6083	0.8890	0.050*
H4B	0.0448	0.5608	0.8387	0.050*
C5	−0.0846 (6)	0.8114 (3)	0.8436 (2)	0.0575 (8)
H5A	−0.2360	0.8978	0.8392	0.069*
H5B	0.0113	0.8527	0.7860	0.069*
C6	0.0179 (4)	0.7906 (3)	0.94565 (19)	0.0389 (5)
C7	−0.1118 (4)	0.8301 (3)	1.0313 (2)	0.0458 (6)
H7	−0.2711	0.8749	1.0242	0.055*
C8	0.1937 (5)	0.7467 (3)	1.1312 (2)	0.0507 (7)
H8	0.2567	0.7298	1.1962	0.061*
C9	0.3376 (4)	0.7045 (3)	1.0513 (2)	0.0460 (6)
H9	0.4963	0.6603	1.0606	0.055*
C10	0.2489 (4)	0.7271 (3)	0.95738 (19)	0.0417 (5)
H10	0.3462	0.6992	0.9005	0.050*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu	0.02142 (18)	0.02502 (19)	0.0296 (2)	−0.00597 (13)	−0.00336 (13)	−0.00873 (14)
N1	0.0370 (10)	0.0319 (10)	0.0332 (10)	−0.0132 (8)	−0.0058 (8)	−0.0086 (8)
N2	0.0266 (8)	0.0378 (10)	0.0292 (9)	−0.0082 (7)	−0.0023 (7)	−0.0121 (8)
N3	0.0777 (16)	0.0397 (12)	0.0397 (13)	−0.0190 (11)	0.0090 (11)	−0.0145 (10)
O1	0.0421 (9)	0.0819 (14)	0.0342 (9)	−0.0235 (9)	0.0035 (7)	−0.0280 (9)
O2	0.0401 (9)	0.0620 (12)	0.0555 (12)	−0.0036 (8)	−0.0106 (8)	−0.0300 (9)
O1W	0.0399 (9)	0.0668 (12)	0.0526 (11)	−0.0158 (8)	0.0015 (8)	−0.0243 (9)
O2W	0.0781 (14)	0.0525 (12)	0.0540 (13)	−0.0063 (10)	0.0207 (11)	−0.0053 (10)
C1	0.0364 (12)	0.0340 (12)	0.0404 (13)	0.0026 (9)	−0.0085 (10)	−0.0078 (10)
C2	0.0478 (13)	0.0284 (11)	0.0425 (14)	−0.0068 (10)	−0.0010 (10)	−0.0129 (10)
C3	0.0380 (12)	0.0386 (12)	0.0311 (12)	−0.0163 (9)	−0.0034 (9)	−0.0119 (9)
C4	0.0532 (14)	0.0418 (13)	0.0336 (13)	−0.0141 (11)	−0.0079 (10)	−0.0126 (10)
C5	0.089 (2)	0.0386 (14)	0.0508 (17)	−0.0225 (14)	−0.0349 (15)	−0.0035 (12)
C6	0.0540 (14)	0.0294 (11)	0.0378 (13)	−0.0159 (10)	−0.0144 (11)	−0.0068 (10)
C7	0.0436 (13)	0.0338 (12)	0.0636 (18)	−0.0142 (10)	−0.0036 (12)	−0.0137 (12)
C8	0.083 (2)	0.0384 (14)	0.0338 (14)	−0.0169 (13)	−0.0209 (13)	−0.0078 (11)
C9	0.0479 (14)	0.0426 (14)	0.0516 (16)	−0.0146 (11)	−0.0149 (12)	−0.0121 (12)
C10	0.0519 (14)	0.0419 (13)	0.0353 (13)	−0.0169 (11)	−0.0005 (10)	−0.0132 (10)

Geometric parameters (Å, º)

Cu—O1W^{i}	2.503 (2)	C1—C2	1.506 (3)
Cu—O1W	2.503 (2)	C1—H1C	0.9900
Cu—N1^{i}	2.015 (2)	C1—H1D	0.9900
Cu—N1	2.015 (2)	C2—H2C	0.9900
Cu—N2^{i}	2.022 (2)	C2—H2D	0.9900
Cu—N2	2.022 (2)	C3—C4	1.521 (3)
O1—C3	1.251 (3)	C4—C5	1.498 (3)
O2—C3	1.250 (3)	C4—H4A	0.9900

O1W—H1W	0.84	C4—H4B	0.9900
O1W—H2W	0.84	C5—C6	1.513 (3)
O2W—H3W	0.84	C5—H5A	0.9900
O2W—H4W	0.84	C5—H5B	0.9900
N1—C2	1.472 (3)	C6—C7	1.378 (4)
N1—H1A	0.9200	C6—C10	1.379 (3)
N1—H1B	0.9200	C7—H7	0.9500
N2—C1	1.480 (3)	C8—C9	1.363 (4)
N2—H2A	0.9200	C8—H8	0.9500
N2—H2B	0.9200	C9—C10	1.370 (3)
N3—C8	1.327 (4)	C9—H9	0.9500
N3—C7	1.337 (4)	C10—H10	0.9500

O1W^{i}—Cu—O1W	180.0	H1C—C1—H1D	108.5
N1^{i}—Cu—O1W^{i}	88.72 (7)	N1—C2—C1	107.48 (18)
N1—Cu—O1W^{i}	91.28 (7)	N1—C2—H2C	110.2
N2^{i}—Cu—O1W^{i}	93.19 (6)	C1—C2—H2C	110.2
N2—Cu—O1W^{i}	86.81 (6)	N1—C2—H2D	110.2
N1^{i}—Cu—O1W	91.28 (7)	C1—C2—H2D	110.2
N1—Cu—O1W	88.72 (7)	H2C—C2—H2D	108.5
N2^{i}—Cu—O1W	86.81 (6)	O2—C3—O1	124.1 (2)
N2—Cu—O1W	93.19 (6)	O2—C3—C4	117.4 (2)
N1^{i}—Cu—N1	180.00 (11)	O1—C3—C4	118.4 (2)
N1^{i}—Cu—N2^{i}	84.91 (7)	C5—C4—C3	113.0 (2)
N1—Cu—N2^{i}	95.09 (7)	C5—C4—H4A	109.0
N1^{i}—Cu—N2	95.09 (7)	C3—C4—H4A	109.0
N1—Cu—N2	84.91 (7)	C5—C4—H4B	109.0
N2^{i}—Cu—N2	180.0	C3—C4—H4B	109.0
C2—N1—Cu	108.14 (13)	H4A—C4—H4B	107.8
C2—N1—H1A	110.1	C4—C5—C6	111.8 (2)
Cu—N1—H1A	110.1	C4—C5—H5A	109.2
C2—N1—H1B	110.1	C6—C5—H5A	109.2
Cu—N1—H1B	110.1	C4—C5—H5B	109.2
H1A—N1—H1B	108.4	C6—C5—H5B	109.2
C1—N2—Cu	107.44 (13)	H5A—C5—H5B	107.9
C1—N2—H2A	110.2	C7—C6—C10	116.7 (2)
Cu—N2—H2A	110.2	C7—C6—C5	122.5 (2)
C1—N2—H2B	110.2	C10—C6—C5	120.8 (2)
Cu—N2—H2B	110.2	N3—C7—C6	124.6 (2)
H2A—N2—H2B	108.5	N3—C7—H7	117.7
C8—N3—C7	116.3 (2)	C6—C7—H7	117.7
Cu—O1W—H1W	110.3	N3—C8—C9	123.8 (2)
Cu—O1W—H2W	104.9	N3—C8—H8	118.1
H1W—O1W—H2W	111.9	C9—C8—H8	118.1
H3W—O2W—H4W	111.2	C8—C9—C10	118.7 (2)
N2—C1—C2	107.81 (18)	C8—C9—H9	120.7
N2—C1—H1C	110.1	C10—C9—H9	120.7
C2—C1—H1C	110.1	C9—C10—C6	119.8 (2)

N2—C1—H1D	110.1	C9—C10—H10	120.1
C2—C1—H1D	110.1	C6—C10—H10	120.1
N2^{i}—Cu—N1—C2	−165.34 (14)	O1—C3—C4—C5	104.8 (3)
N2—Cu—N1—C2	14.66 (14)	C3—C4—C5—C6	−178.5 (2)
O1W^{i}—Cu—N1—C2	101.34 (14)	C4—C5—C6—C7	−96.9 (3)
O1W—Cu—N1—C2	−78.66 (14)	C4—C5—C6—C10	81.8 (3)
N1^{i}—Cu—N2—C1	−165.31 (14)	C8—N3—C7—C6	−0.2 (4)
N1—Cu—N2—C1	14.70 (14)	C10—C6—C7—N3	−0.5 (4)
O1W^{i}—Cu—N2—C1	−76.88 (14)	C5—C6—C7—N3	178.2 (2)
O1W—Cu—N2—C1	103.12 (14)	C7—N3—C8—C9	0.7 (4)
Cu—N2—C1—C2	−40.8 (2)	N3—C8—C9—C10	−0.4 (4)
Cu—N1—C2—C1	−40.7 (2)	C8—C9—C10—C6	−0.4 (4)
N2—C1—C2—N1	54.5 (2)	C7—C6—C10—C9	0.8 (3)
O2—C3—C4—C5	−77.7 (3)	C5—C6—C10—C9	−178.0 (2)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O2^{ii}	0.92	2.32	3.130 (3)	147
N1—H1*A*···O1^{ii}	0.92	2.41	3.247 (2)	152
N1—H1*B*···O2*W*	0.92	2.11	2.944 (3)	151
N2—H2*A*···O1^{iii}	0.92	2.29	3.150 (3)	155
N2—H2*B*···O1	0.92	2.12	3.019 (2)	164
O1*W*—H1*W*···O2^{ii}	0.84	2.06	2.873 (3)	164
O1*W*—H2*W*···O1	0.84	2.00	2.814 (2)	164
O2*W*—H3*W*···N3^{iv}	0.84	2.08	2.899 (3)	163
O2*W*—H4*W*···O2^{v}	0.84	2.03	2.859 (3)	169

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