Aqua[1-(4-carboxyphenyl)-1*H*-imidazole-κN^3](pyridine-2,6-dicarboxylato-$\kappa^3 O^2$,*N*,O^6)copper(II) monohydrate

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In the title complex, [Cu(C₇H₃NO₄)(C₁₀H₈N₂O₂)(H₂O)]·H₂O, the Cu^{II} ion is in a slightly distorted square-pyramidal geometry. Two carboxylate O atoms and one pyridine N atom from a pyridine-2,6-dicarboxylate ligand chelate the Cu^{II} ion, forming two stable five-membered metalla rings. One imidazole N atom from a 1-(4-carboxyphenyl)imidazole ligand and one water molecule complete the five-coordination. O—H···O hydrogen bonds involving the coordinated water molecules and carboxylate groups link the complex molecules into chain-containing dinuclear macrocycles. O—H···O hydrogen bonds involving the uncoordinated water molecules link the chains into a layer extending parallel to (10$\bar{1}$).

Related literature

For the design and synthesis of compounds with metal–organic supramolecular architectures, see: Bradshaw *et al.* (2005); Tian *et al.* (2005); Wang *et al.* (2009). For the use of N-containing heterocyclic carboxylate ligands in metal–organic supramolecular architectures, see: Bentiss *et al.* (2004); Yang *et al.* (2008); Zeng *et al.* (2006). For related structures, see: Li *et al.* (2008).
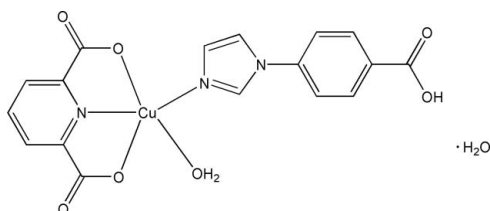
Experimental

Crystal data

[Cu(C₇H₃NO₄)(C₁₀H₈N₂O₂)(H₂O)]·H₂O
$M_r = 452.87$
Triclinic, $P\bar{1}$

$a = 8.1638$ (5) Å
$b = 8.2081$ (5) Å
$c = 13.1265$ (18) Å
$\alpha = 84.353$ (16)°
$\beta = 85.789$ (13)°
$\gamma = 80.736$ (14)°

$V = 862.43$ (15) Å³
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 1.32$ mm^{-1}
$T = 293$ K
$0.34 \times 0.20 \times 0.15$ mm

Data collection

Bruker APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.662$, $T_{max} = 0.826$

6749 measured reflections
3920 independent reflections
3485 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.096$
$S = 1.06$
3920 reflections
322 parameters
5 restraints

H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.62$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O3^i	0.81 (1)	1.90 (1)	2.710 (2)	173 (4)
O1W—H1W1···O2W^{ii}	0.82 (2)	2.02 (2)	2.803 (3)	159 (4)
O1W—H2W1···O5^{ii}	0.82 (2)	1.92 (2)	2.740 (2)	177 (3)
O2W—H1W2···O6	0.83 (2)	1.98 (2)	2.794 (3)	168 (3)
O2W—H2W2···O2^{iii}	0.83 (2)	2.25 (2)	2.986 (3)	148 (3)

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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supporting information

Aqua[1-(4-carboxyphenyl)-1*H*-imidazole-*κN³*](pyridine-2,6-dicarboxylato-*κ³O²,N,O⁶*)copper(II) monohydrate

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S1. Comment

The rational design and synthesis of metal–organic supramolecular architectures are of great interest and importance owing to their intriguing structural topologies and potential applications as functional materials (Bradshaw *et al.*, 2005). A successful strategy in building the architectures is the deliberate selection of functional organic ligands and transition metal ions with specific coordination geometry. In the context, the carboxylate ligands are widely employed because they exhibit diverse coordination modes (Tian *et al.*, 2005; Wang *et al.*, 2009). The different coordination modes of carboxylate groups can induce different coordination geometries of transition metal ions and enhance the robustness of the resulting architectures. Moreover, the negative charge of carboxylate groups compensates the positive charge from metal ions and can mitigate the counterion effect in self-assembly processes. With the development of supramolecular chemistry and crystal engineering, the scope of the investigations on carboxylate ligands has been widen by the use of N-containing heterocyclic carboxylate ligands, such as pyrazole- (Bentiss *et al.*, 2004), imidazole- (Zeng *et al.*, 2006) and pyridine-carboxylates (Wang *et al.*, 2009; Yang *et al.*, 2008). The introduction of N atoms can satisfy the coordination requirements of metal ions and they also link metal–carboxylate frameworks into various fascinating extended networks. On the other hand, N atoms are highly accessible to transition metal ions, their stronger coordination ability than carboxylate groups may result in the formation of hydrogen bonding interactions by uncoordinated carboxylate O atoms, which further make the whole framework more stable. Among N–containing carboxylate ligands, we are interested in pyridine-2,6-dicarboxylic acid (2,6-H_2pydc) since its N atom and two carboxylate groups may chelate one metal ion, forming two stable five-membered rings (Li *et al.*, 2008). The introduction of the other N-containing carboxylate ligands may lead to interesting structural frameworks. Herein, we report a Cu(II) supramolecular complex from 2,6-H_2pydc and 4-(imidazol-1-yl)benzoic acid (HIBA).

As shown in Fig. 1, the Cu^{II} ion has a slightly distorted square-pyramidal coordination geometry. Two carboxylate O atoms and one pyridine N atom from a 2,6-pydc ligand and one imidazolyl N atom from HIBA are in the basal plane, with a mean deviation of 0.0222 (2) Å from the plane. Cu1 atom is slightly out of the plane about 0.2221 (3) Å. One water molecule (O1W) occupies the apical position. As expected, two O atoms (O4, O6) from different carboxylate groups and an N atom (N3) chelate Cu1, forming two stable five-membered rings. This results in Cu1—N3 bond distance of 1.9075 (17) Å being much shorter than Cu1—N1 bond distance of 1.9467 (18) Å. Two carboxylate groups (O3, O4, C11 and O5, O6, C17) are almost coplanar with the pyridine ring, with dihedral angles between them of 3.5 (1) and 7.3 (2)°, respectively. HIBA serves as a monodentate ligand through imidazolyl N atom coordinating to Cu1 atom. The twisting angle between the imidazolyl ring and benzene ring is 23.02 (8)°, while the dihedral angle between the benzene ring and the carboxylate group in HIBA is 2.7 (2)°.

Interestingly, carboxylic proton forms a strong hydrogen bond with one uncoordinated carboxylate O atom of the 2,6-pydc ligand (Table 1), which results in a dinuclear supramolecular macrocycle (Fig. 2). The Cu···Cu separation in the cycle is 13.749 (2) Å. O—H···O hydrogen bonds between the other carboxylate group of the 2,6-pydc ligand and the coordinated water molecule link the macrocyles into a one-dimensional supramolecular chain (Fig. 3). The nearest Cu···Cu separation in the chain is 6.322 (1) Å. O—H···O hydrogen bonds involving the uncoordinated water molecules link the chains into a layer.

S2. Experimental

A mixture of pyridine-2,6-dicarboxylic acid (0.034 g, 0.2 mmol), HIBA (0.038 g, 0.2 mmol), copper nitrate hydrate (0.036 g, 0.2 mmol) and one drop of KOH aqueous solution (10%) in 15 ml distilled water was heated in a 30 ml Teflon-lined steel bomb at 433 K for 3 d. Blue crystals formed were collected, washed with ethanol and dried in air.

S3. Refinement

All H atoms were located from difference Fourier maps and refined isotropically, with a distance restraint of O—H = 0.82 (1) Å.
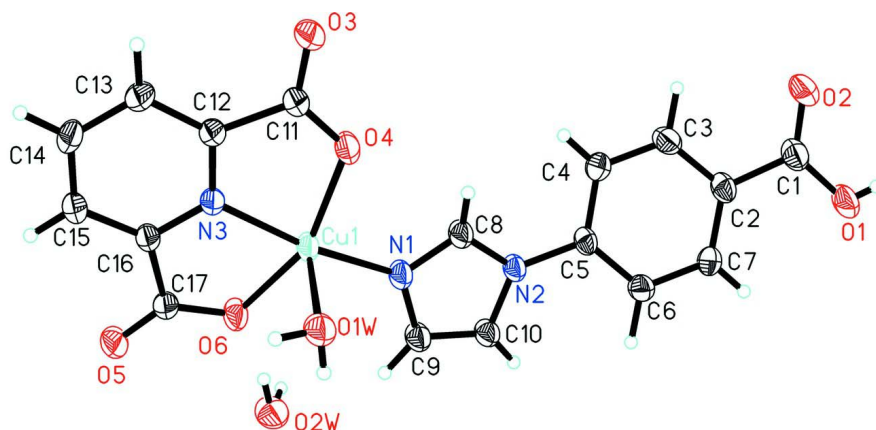

Figure 1

Molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.
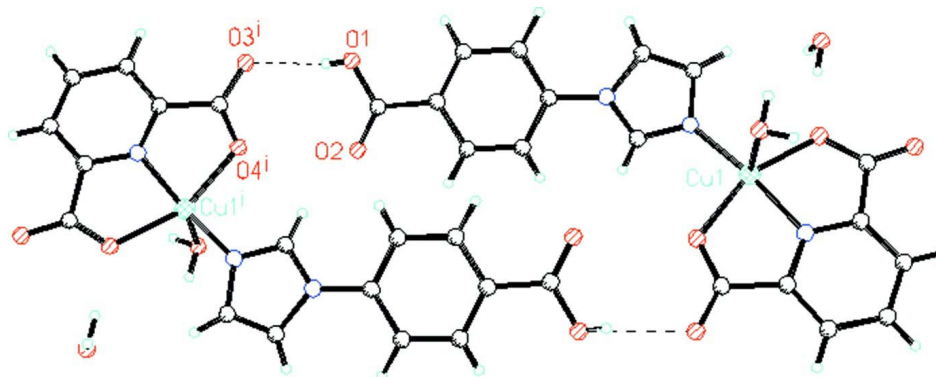

Figure 2

View of the dinuclear Cu^{II} supramolecular macrocycle. Dashed lines denote hydrogen bonds. [Symmetry code: (i) -x, -y+1, -z+1.]
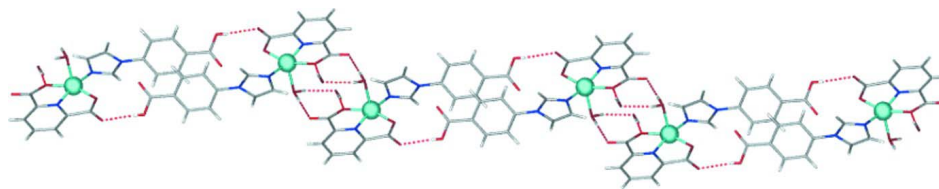
Figure 3
View of the one-dimensional supramolecular chain. Dashed lines denote hydrogen bonds.

Aqua[1-(4-carboxyphenyl)-1*H*-imidazole-κN^3](pyridine- 2,6-dicarboxylato-$\kappa^3 O^2$,*N*,O^6)copper(II) monohydrate

Crystal data

[Cu(C$_7$H$_3$NO$_4$)(C$_{10}$H$_8$N$_2$O$_2$)(H$_2$O)]·H$_2$O	$Z = 2$
$M_r = 452.87$	$F(000) = 462$
Triclinic, $P\bar{1}$	$D_x = 1.744$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 8.1638$ (5) Å	Cell parameters from 6749 reflections
$b = 8.2081$ (5) Å	$\theta = 2.9–27.5°$
$c = 13.1265$ (18) Å	$\mu = 1.32$ mm^{-1}
$\alpha = 84.353$ (16)°	$T = 293$ K
$\beta = 85.789$ (13)°	Block, blue
$\gamma = 80.736$ (14)°	$0.34 \times 0.20 \times 0.15$ mm
$V = 862.43$ (15) Å^3	

Data collection

Bruker APEX CCD diffractometer	6749 measured reflections
Radiation source: fine-focus sealed tube	3920 independent reflections
Graphite monochromator	3485 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.020$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$\theta_{max} = 27.5°$, $\theta_{min} = 2.9°$
	$h = -10\rightarrow10$
	$k = -10\rightarrow10$
$T_{min} = 0.662$, $T_{max} = 0.826$	$l = -14\rightarrow17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.036$	
$wR(F^2) = 0.096$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.06$	
3920 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0513P)^2 + 0.3344P]$ where $P = (F_o^2 + 2F_c^2)/3$
322 parameters	
5 restraints	$(\Delta/\sigma)_{max} = 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 0.37$ e Å^{-3}
	$\Delta\rho_{min} = -0.62$ e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}
Cu1	0.51191 (3)	0.77853 (3)	0.81495 (2)	0.02775 (11)
O1	−0.5172 (2)	0.7396 (3)	0.42103 (17)	0.0516 (5)
N1	0.3000 (2)	0.8750 (2)	0.75900 (14)	0.0286 (4)

C1	−0.3561 (3)	0.6898 (3)	0.40439 (19)	0.0347 (5)
H1	−0.575 (4)	0.708 (5)	0.381 (2)	0.076 (12)*
O2	−0.2974 (2)	0.6052 (3)	0.33628 (16)	0.0533 (5)
N2	0.0788 (2)	0.8924 (2)	0.67065 (13)	0.0245 (4)
C2	−0.2492 (3)	0.7482 (3)	0.47641 (17)	0.0283 (5)
O3	0.7305 (2)	0.3533 (2)	0.70285 (15)	0.0414 (4)
N3	0.7383 (2)	0.6954 (2)	0.84101 (14)	0.0244 (4)
C3	−0.0783 (3)	0.6968 (3)	0.46374 (18)	0.0312 (5)
H3	−0.036 (4)	0.627 (4)	0.408 (2)	0.046 (8)*
O4	0.5460 (2)	0.5751 (2)	0.73733 (14)	0.0376 (4)
C4	0.0295 (3)	0.7460 (3)	0.52654 (18)	0.0300 (5)
H4	0.135 (4)	0.714 (3)	0.515 (2)	0.038 (7)*
O5	0.7779 (2)	1.0466 (2)	0.96052 (14)	0.0392 (4)
C5	−0.0332 (3)	0.8478 (2)	0.60358 (16)	0.0237 (4)
O6	0.57541 (19)	0.97815 (19)	0.87486 (13)	0.0333 (4)
C6	−0.2030 (3)	0.9038 (3)	0.61558 (17)	0.0290 (4)
H6	−0.247 (3)	0.981 (3)	0.673 (2)	0.039 (7)*
C7	−0.3103 (3)	0.8539 (3)	0.55223 (18)	0.0305 (5)
H7	−0.418 (4)	0.888 (3)	0.562 (2)	0.036 (7)*
C8	0.2294 (3)	0.8052 (3)	0.69116 (17)	0.0282 (4)
H8	0.265 (3)	0.706 (3)	0.6699 (18)	0.026 (6)*
C9	0.1899 (3)	1.0144 (3)	0.78355 (18)	0.0290 (5)
H9	0.213 (3)	1.084 (3)	0.830 (2)	0.030 (6)*
C10	0.0526 (3)	1.0255 (3)	0.72996 (17)	0.0280 (4)
H10	−0.043 (3)	1.102 (3)	0.726 (2)	0.033 (7)*
C11	0.6874 (3)	0.4845 (3)	0.74368 (17)	0.0291 (5)
C12	0.8070 (3)	0.5506 (3)	0.80631 (17)	0.0255 (4)
C13	0.9705 (3)	0.4866 (3)	0.82600 (19)	0.0309 (5)
H13	1.023 (4)	0.383 (4)	0.803 (2)	0.052 (8)*
C14	1.0569 (3)	0.5759 (3)	0.88262 (19)	0.0324 (5)
H14	1.165 (4)	0.537 (4)	0.895 (2)	0.049 (8)*
C15	0.9826 (3)	0.7273 (3)	0.91638 (18)	0.0287 (4)
H15	1.038 (3)	0.791 (3)	0.955 (2)	0.037 (7)*
C16	0.8205 (3)	0.7846 (3)	0.89290 (16)	0.0240 (4)
C17	0.7182 (3)	0.9512 (3)	0.91352 (17)	0.0269 (4)
O1W	0.4032 (2)	0.6744 (2)	0.96552 (14)	0.0357 (4)
O2W	0.3880 (2)	1.2940 (2)	0.87970 (16)	0.0427 (4)
H1W1	0.474 (4)	0.658 (5)	1.008 (2)	0.074 (12)*
H2W1	0.349 (4)	0.756 (3)	0.990 (2)	0.055 (9)*
H1W2	0.445 (4)	1.203 (3)	0.869 (2)	0.054 (9)*
H2W2	0.396 (4)	1.341 (4)	0.8208 (17)	0.061 (11)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.02014 (15)	0.02746 (16)	0.03696 (18)	0.00146 (10)	−0.01098 (11)	−0.01095 (11)
O1	0.0321 (10)	0.0655 (13)	0.0633 (13)	0.0001 (9)	−0.0194 (9)	−0.0361 (11)
N1	0.0232 (9)	0.0299 (9)	0.0334 (10)	0.0004 (7)	−0.0105 (7)	−0.0080 (7)

C1	0.0339 (12)	0.0319 (12)	0.0404 (13)	−0.0037 (9)	−0.0120 (10)	−0.0084 (10)
O2	0.0403 (10)	0.0672 (13)	0.0592 (13)	−0.0047 (9)	−0.0134 (9)	−0.0379 (11)
N2	0.0224 (8)	0.0254 (9)	0.0266 (9)	−0.0013 (7)	−0.0083 (7)	−0.0049 (7)
C2	0.0292 (11)	0.0288 (11)	0.0283 (11)	−0.0037 (9)	−0.0113 (9)	−0.0029 (8)
O3	0.0322 (9)	0.0394 (9)	0.0561 (11)	0.0020 (7)	−0.0108 (8)	−0.0277 (8)
N3	0.0204 (8)	0.0244 (8)	0.0293 (9)	−0.0010 (7)	−0.0051 (7)	−0.0077 (7)
C3	0.0335 (12)	0.0317 (11)	0.0290 (11)	−0.0005 (9)	−0.0074 (9)	−0.0092 (9)
O4	0.0268 (8)	0.0371 (9)	0.0522 (10)	0.0015 (7)	−0.0155 (7)	−0.0211 (8)
C4	0.0224 (10)	0.0351 (12)	0.0325 (11)	0.0003 (9)	−0.0063 (9)	−0.0073 (9)
O5	0.0319 (9)	0.0365 (9)	0.0534 (11)	−0.0019 (7)	−0.0107 (8)	−0.0240 (8)
C5	0.0238 (10)	0.0247 (10)	0.0232 (10)	−0.0031 (8)	−0.0087 (8)	−0.0012 (8)
O6	0.0265 (8)	0.0262 (8)	0.0488 (10)	0.0031 (6)	−0.0151 (7)	−0.0131 (7)
C6	0.0258 (10)	0.0341 (11)	0.0273 (11)	0.0003 (9)	−0.0065 (8)	−0.0074 (9)
C7	0.0214 (10)	0.0391 (12)	0.0318 (11)	−0.0018 (9)	−0.0070 (9)	−0.0074 (9)
C8	0.0238 (10)	0.0287 (11)	0.0326 (11)	0.0021 (8)	−0.0104 (8)	−0.0084 (9)
C9	0.0278 (11)	0.0257 (10)	0.0340 (12)	0.0001 (8)	−0.0097 (9)	−0.0073 (9)
C10	0.0264 (11)	0.0259 (10)	0.0321 (11)	0.0006 (9)	−0.0083 (9)	−0.0075 (8)
C11	0.0248 (10)	0.0319 (11)	0.0327 (11)	−0.0037 (9)	−0.0055 (9)	−0.0120 (9)
C12	0.0224 (10)	0.0255 (10)	0.0294 (11)	−0.0021 (8)	−0.0038 (8)	−0.0077 (8)
C13	0.0244 (11)	0.0280 (11)	0.0397 (13)	0.0038 (9)	−0.0053 (9)	−0.0097 (9)
C14	0.0202 (10)	0.0355 (12)	0.0413 (13)	0.0017 (9)	−0.0085 (9)	−0.0071 (10)
C15	0.0250 (10)	0.0328 (11)	0.0303 (11)	−0.0055 (9)	−0.0074 (9)	−0.0068 (9)
C16	0.0216 (9)	0.0242 (10)	0.0272 (10)	−0.0030 (8)	−0.0050 (8)	−0.0060 (8)
C17	0.0229 (10)	0.0274 (10)	0.0314 (11)	−0.0019 (8)	−0.0043 (8)	−0.0085 (8)
O1W	0.0334 (9)	0.0336 (9)	0.0407 (10)	0.0007 (7)	−0.0077 (8)	−0.0119 (7)
O2W	0.0458 (11)	0.0343 (10)	0.0467 (11)	0.0060 (8)	−0.0110 (9)	−0.0103 (8)

Geometric parameters (Å, º)

Cu1—N1	1.9467 (18)	O5—C17	1.222 (3)
Cu1—N3	1.9076 (17)	C5—C6	1.391 (3)
Cu1—O4	2.0118 (16)	O6—C17	1.283 (3)
Cu1—O6	2.0393 (16)	C6—C7	1.385 (3)
Cu1—O1W	2.2537 (19)	C6—H6	1.04 (3)
O1—C1	1.322 (3)	C7—H7	0.88 (3)
O1—H1	0.81 (1)	C8—H8	0.89 (3)
N1—C8	1.318 (3)	C9—C10	1.353 (3)
N1—C9	1.386 (3)	C9—H9	0.92 (3)
C1—O2	1.210 (3)	C10—H10	0.92 (3)
C1—C2	1.493 (3)	C11—C12	1.517 (3)
N2—C8	1.350 (3)	C12—C13	1.386 (3)
N2—C10	1.383 (3)	C13—C14	1.392 (3)
N2—C5	1.426 (3)	C13—H13	0.95 (3)
C2—C3	1.393 (3)	C14—C15	1.391 (3)
C2—C7	1.396 (3)	C14—H14	0.91 (3)
O3—C11	1.239 (3)	C15—C16	1.378 (3)
N3—C16	1.332 (3)	C15—H15	0.95 (3)
N3—C12	1.337 (3)	C16—C17	1.521 (3)

C3—C4	1.379 (3)	O1W—H1W1	0.82 (2)
C3—H3	0.98 (3)	O1W—H2W1	0.82 (2)
O4—C11	1.272 (3)	O2W—H1W2	0.83 (2)
C4—C5	1.391 (3)	O2W—H2W2	0.83 (2)
C4—H4	0.87 (3)		
N3—Cu1—N1	167.81 (8)	C5—C6—H6	119.4 (16)
N3—Cu1—O4	80.11 (7)	C6—C7—C2	120.5 (2)
N1—Cu1—O4	95.85 (7)	C6—C7—H7	118.2 (18)
N3—Cu1—O6	80.22 (7)	C2—C7—H7	121.3 (18)
N1—Cu1—O6	100.91 (7)	N1—C8—N2	110.75 (19)
O4—Cu1—O6	156.95 (7)	N1—C8—H8	125.3 (16)
N3—Cu1—O1W	96.05 (7)	N2—C8—H8	123.1 (16)
N1—Cu1—O1W	95.97 (8)	C10—C9—N1	109.0 (2)
O4—Cu1—O1W	99.71 (7)	C10—C9—H9	128.9 (16)
O6—Cu1—O1W	94.19 (7)	N1—C9—H9	122.2 (16)
C1—O1—H1	114 (3)	C9—C10—N2	106.46 (19)
C8—N1—C9	106.55 (18)	C9—C10—H10	132.6 (17)
C8—N1—Cu1	123.09 (15)	N2—C10—H10	120.9 (17)
C9—N1—Cu1	130.21 (15)	O3—C11—O4	125.2 (2)
O2—C1—O1	123.7 (2)	O3—C11—C12	120.44 (19)
O2—C1—C2	121.8 (2)	O4—C11—C12	114.40 (18)
O1—C1—C2	114.5 (2)	N3—C12—C13	119.5 (2)
C8—N2—C10	107.26 (18)	N3—C12—C11	111.02 (18)
C8—N2—C5	125.26 (18)	C13—C12—C11	129.41 (19)
C10—N2—C5	127.41 (18)	C12—C13—C14	118.2 (2)
C3—C2—C7	119.1 (2)	C12—C13—H13	122 (2)
C3—C2—C1	117.1 (2)	C14—C13—H13	119.8 (19)
C7—C2—C1	123.8 (2)	C15—C14—C13	120.9 (2)
C16—N3—C12	123.10 (18)	C15—C14—H14	119.7 (19)
C16—N3—Cu1	118.33 (14)	C13—C14—H14	119.3 (19)
C12—N3—Cu1	118.58 (15)	C16—C15—C14	117.7 (2)
C4—C3—C2	120.8 (2)	C16—C15—H15	119.2 (17)
C4—C3—H3	120.8 (18)	C14—C15—H15	123.0 (17)
C2—C3—H3	118.4 (18)	N3—C16—C15	120.51 (19)
C11—O4—Cu1	115.70 (14)	N3—C16—C17	111.96 (18)
C3—C4—C5	119.6 (2)	C15—C16—C17	127.41 (19)
C3—C4—H4	117.9 (19)	O5—C17—O6	126.6 (2)
C5—C4—H4	122.4 (19)	O5—C17—C16	119.27 (19)
C6—C5—C4	120.4 (2)	O6—C17—C16	114.11 (18)
C6—C5—N2	120.54 (18)	Cu1—O1W—H1W1	110 (3)
C4—C5—N2	119.10 (19)	Cu1—O1W—H2W1	104 (2)
C17—O6—Cu1	114.41 (13)	H1W1—O1W—H2W1	96 (3)
C7—C6—C5	119.6 (2)	H1W2—O2W—H2W2	98 (3)
C7—C6—H6	121.0 (16)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O3[i]	0.81 (1)	1.90 (1)	2.710 (2)	173 (4)
O1*W*—H1*W*1···O2*W*[ii]	0.82 (2)	2.02 (2)	2.803 (3)	159 (4)
O1*W*—H2*W*1···O5[ii]	0.82 (2)	1.92 (2)	2.740 (2)	177 (3)
O2*W*—H1*W*2···O6	0.83 (2)	1.98 (2)	2.794 (2)	168 (3)
O2*W*—H2*W*2···O2[iii]	0.83 (2)	2.25 (2)	2.986 (3)	148 (3)

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