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Aqua(2,2′-biimidazole)(pyridine-2,6-dicarboxylato)copper(II) monohydrate

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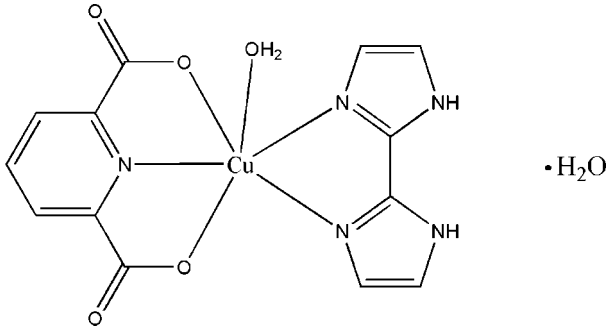
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.006 Å; R factor = 0.049; wR factor = 0.148; data-to-parameter ratio = 12.2.

In the title compound, $[Cu(C_7H_3NO_4)(C_6H_6N_4)(H_2O)]\cdot H_2O$, the central Cu^{II} ion exhibits a distorted *mer*-CuN_3O_3 octahedral geometry arising from one water O atom, an *N*,*N*-bidentate 2,2′-biimidazole molecule and an *N*,*O*,*O*-tridentate pyridine-2,6-dicarboxylate dianion. The crystal packing is stabilized by O—H···O, N—H···O and C—H···O hydrogen bonds.

Related literature

For related literature, see: Whitesides *et al.* (1991); Rebek (1990); Xiao & Shreeve (2005).



Experimental

Crystal data

$[Cu(C_7H_3NO_4)(C_6H_6N_4)(H_2O)]\cdot H_2O$
M_r = 398.82
Triclinic, $P\overline{1}$
a = 6.5951 (4) Å
b = 10.6971 (7) Å
c = 11.6112 (7) Å
α = 97.210 (1)°
β = 94.384 (1)°
γ = 106.411 (1)°
V = 774.16 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.46 mm^{-1}
T = 296 (2) K
0.35 × 0.10 × 0.06 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.630, T_{max} = 0.918
7976 measured reflections
2978 independent reflections
2595 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.148
S = 1.10
2978 reflections
244 parameters
8 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.82 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—N1	1.974 (3)	Cu1—N2	2.100 (3)
Cu1—N4	2.056 (3)	Cu1—O3	2.120 (3)
Cu1—O5	2.076 (3)	Cu1—O1	2.141 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
O6—H6A···O3^{i}	0.84 (3)	1.90 (4)	2.700 (5)	160 (9)
O5—H5B···O6^{ii}	0.84 (3)	1.88 (3)	2.719 (5)	174 (5)
O5—H5A···O4^{iii}	0.80 (3)	2.01 (3)	2.813 (4)	175 (5)
N5—H5C···O2^{iv}	0.83 (3)	2.05 (3)	2.871 (5)	166 (4)
N3—H3A···O1^{iv}	0.83 (3)	1.97 (3)	2.729 (4)	152 (4)
C3—H3···O6	0.93	2.55	3.359 (6)	146
C13—H13···O2^{v}	0.93	2.43	3.298 (5)	156
C4—H4···O4^{vi}	0.93	2.48	3.294 (5)	147

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

We thank Xianggao Meng for assistance.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2508).

References

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supplementary materials

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Aqua(2,2'-biimidazole)(pyridine-2,6-dicarboxylato)copper(II) monohydrate

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Comment

Biimidazole (H_2biim) is a bidentate chelating ligand with multiple proton-donor sites which can coordinate to a transition metal in its neutral (H_2biim), singly-deprotonated ($Hbiim^-$) and doubly-deprotonated ($biim^{2-}$) forms. Coordinated H_2biim usually forms hydrogen bonds with counteranions or solvent molecules (Whitesides *et al.*, (1991); Rebek,1990).

Here, we report the synthesis and sructure of the the title compound, (I), which contains Cu(II) ions, neutral H_2biim and pyridine-2,6-dicarboxylate (pda) dianions. The Cu^{II} ion in (I) exhibits a distorted *mer*-CuN_3O_3 octahedral geometry (Table 1), arising from N1, N2, N4 and O5 as equatorial atoms and O1 and O3 as axial atoms.

The packing for (I) is mainly governed by a combination of O(or N, C)–H···O hydrogen bonds (Table 2, Fig. 2) linking the constituent species together.

Experimental

2,2'-biimidazole was synthesized according to the literature procedure (Xiao & Shreeve, 2005). A mixture of $Cu(NO_3)_2{\cdot}4H_2O$, pyridine-2,6-dicarboxylic acid, 2,2'-biimidazole and water in a molar ratio of 1:1:1:555 was sealed in a 23 ml polyfluoroethylene-lined stainless steel bomb and heated to 423 K under autogenous pressure for 72 h. After slowly cooling to room temperature and opening the bomb, blue plates of (I) were formed, collected by filtration, washed in de-ionized water, and finally dried.

Refinement

The N– and O-bound H atoms were located in difference maps and refined with distance restraints [N–H = 0.86 (3) Å, O–H = 0.85 (3) Å, H···H = 1.39 (3) Å] and the constraints U_{iso}(H) = 1.2U_{eq}(N) or 1.5U_{eq}(O).

The C-bound H atoms were geometrically placed (C—H = 0.93 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C).

Figures

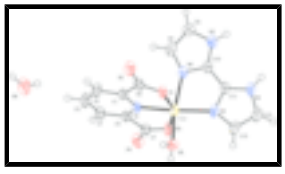

Fig. 1. View of the molecular structure of (I), showing 50% probability displacement ellipsoids for the non-hydrogen atoms.

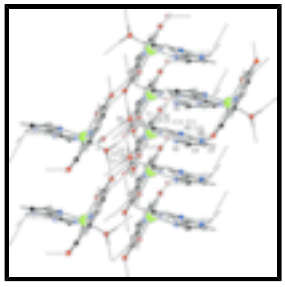

Fig. 2. Part of the crystal structure of (I) showing the formation of the two-dimensinal network. Hydrogen bonds are shown as dashed lines.

Aqua(2,2'-biimidazole)(pyridine-2,6-dicarboxylato)copper(II) monohydrate

Crystal data

$[Cu(C_7H_3NO_4)(C_6H_6N_4)(H_2O)]\cdot H_2O$	$Z = 2$
$M_r = 398.82$	$F_{000} = 406$
Triclinic, $P\overline{1}$	$D_x = 1.711$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 6.5951$ (4) Å	Cell parameters from 3382 reflections
$b = 10.6971$ (7) Å	$\theta = 2.5$–27.8°
$c = 11.6112$ (7) Å	$\mu = 1.46$ mm^{-1}
$\alpha = 97.210$ (1)°	$T = 296$ (2) K
$\beta = 94.384$ (1)°	Plate, blue
$\gamma = 106.411$ (1)°	0.35 × 0.10 × 0.06 mm
$V = 774.16$ (8) Å^3	

Data collection

Bruker SMART CCD diffractometer	2978 independent reflections
Radiation source: fine-focus sealed tube	2595 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.029$
$T = 296(2)$ K	$\theta_{max} = 26.0^\circ$
ω scans	$\theta_{min} = 1.8^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2001)	$h = -8\rightarrow8$
$T_{min} = 0.630$, $T_{max} = 0.918$	$k = -13\rightarrow13$
7976 measured reflections	$l = -14\rightarrow12$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.049$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.148$	$w = 1/[\sigma^2(F_o^2) + (0.0837P)^2 + 1.1035P]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 1.10	$(\Delta/\sigma)_{max} < 0.001$
2978 reflections	$\Delta\rho_{max}$ = 0.82 e Å^{-3}
244 parameters	$\Delta\rho_{min}$ = −0.52 e Å^{-3}
8 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.72700 (7)	0.86989 (4)	0.73050 (4)	0.0290 (2)
C1	0.6942 (6)	0.5957 (3)	0.7217 (3)	0.0269 (8)
C2	0.5990 (7)	0.4613 (4)	0.6989 (4)	0.0376 (10)
H2	0.6697	0.4032	0.7225	0.045*
C3	0.3954 (7)	0.4149 (4)	0.6399 (4)	0.0411 (10)
H3	0.3290	0.3245	0.6229	0.049*
C4	0.2892 (6)	0.5014 (4)	0.6059 (4)	0.0345 (9)
H4	0.1518	0.4711	0.5670	0.041*
C5	0.3952 (6)	0.6344 (3)	0.6320 (3)	0.0261 (8)
C6	0.9129 (6)	0.6668 (4)	0.7889 (3)	0.0277 (8)
C7	0.3065 (6)	0.7458 (4)	0.6035 (3)	0.0281 (8)
C8	0.5874 (6)	0.7965 (4)	0.9848 (4)	0.0348 (9)
H8	0.5183	0.7064	0.9679	0.042*
C9	0.6372 (6)	0.8679 (4)	1.0932 (4)	0.0341 (9)
H9	0.6103	0.8369	1.1635	0.041*
C10	0.7441 (5)	0.9956 (3)	0.9642 (3)	0.0252 (8)
C11	0.8339 (5)	1.1019 (3)	0.9001 (3)	0.0266 (8)
C12	0.9225 (6)	1.1865 (4)	0.7462 (4)	0.0348 (9)
H12	0.9476	1.1949	0.6694	0.042*
C13	0.9615 (7)	1.2875 (4)	0.8357 (4)	0.0379 (10)
H13	1.0156	1.3769	0.8315	0.046*
N1	0.5914 (5)	0.6780 (3)	0.6882 (3)	0.0240 (6)
N2	0.6540 (5)	0.8769 (3)	0.9036 (3)	0.0286 (7)
N4	0.8402 (5)	1.0698 (3)	0.7868 (3)	0.0292 (7)
N3	0.7358 (5)	0.9956 (3)	1.0784 (3)	0.0301 (7)
H3A	0.789 (7)	1.059 (3)	1.131 (3)	0.036*

N5	0.9061 (5)	1.2329 (3)	0.9335 (3)	0.0296 (7)
H5C	0.908 (7)	1.274 (4)	1.000 (3)	0.036*
O1	0.9727 (4)	0.7904 (2)	0.7902 (2)	0.0286 (6)
O2	1.0086 (5)	0.6037 (3)	0.8420 (3)	0.0425 (8)
O3	0.4277 (4)	0.8609 (3)	0.6434 (3)	0.0380 (7)
O4	0.1318 (5)	0.7184 (3)	0.5452 (3)	0.0406 (7)
O5	0.8806 (5)	0.8899 (3)	0.5814 (3)	0.0366 (7)
H5A	0.957 (7)	0.844 (5)	0.569 (4)	0.055*
H5B	0.808 (7)	0.895 (5)	0.520 (3)	0.055*
O6	0.3788 (10)	0.0955 (4)	0.6068 (4)	0.0869 (16)
H6A	0.378 (13)	0.025 (4)	0.632 (7)	0.130*
H6B	0.480 (10)	0.158 (5)	0.639 (7)	0.130*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0276 (3)	0.0193 (3)	0.0376 (3)	0.00591 (19)	−0.0040 (2)	0.0020 (2)
C1	0.031 (2)	0.0192 (16)	0.0275 (19)	0.0061 (14)	−0.0043 (15)	0.0013 (14)
C2	0.038 (2)	0.0214 (18)	0.053 (3)	0.0122 (17)	−0.0073 (19)	0.0037 (18)
C3	0.039 (2)	0.0196 (18)	0.057 (3)	0.0010 (17)	−0.007 (2)	0.0006 (18)
C4	0.029 (2)	0.0236 (18)	0.042 (2)	0.0003 (15)	−0.0056 (17)	−0.0038 (17)
C5	0.0279 (19)	0.0209 (17)	0.0274 (19)	0.0065 (14)	−0.0038 (15)	0.0015 (14)
C6	0.0250 (18)	0.0266 (18)	0.031 (2)	0.0103 (15)	−0.0012 (15)	−0.0026 (15)
C7	0.0277 (19)	0.0259 (18)	0.033 (2)	0.0121 (15)	0.0000 (16)	0.0039 (15)
C8	0.029 (2)	0.0257 (19)	0.049 (3)	0.0062 (16)	0.0053 (18)	0.0071 (18)
C9	0.027 (2)	0.037 (2)	0.041 (2)	0.0114 (17)	0.0029 (17)	0.0113 (18)
C10	0.0174 (16)	0.0228 (17)	0.036 (2)	0.0088 (13)	−0.0022 (14)	0.0036 (15)
C11	0.0197 (17)	0.0188 (16)	0.039 (2)	0.0060 (13)	−0.0024 (15)	−0.0001 (15)
C12	0.033 (2)	0.0236 (18)	0.046 (2)	0.0059 (16)	−0.0005 (18)	0.0088 (17)
C13	0.035 (2)	0.0228 (19)	0.052 (3)	0.0047 (16)	−0.0067 (19)	0.0087 (18)
N1	0.0237 (15)	0.0190 (14)	0.0272 (16)	0.0061 (12)	−0.0032 (12)	0.0000 (12)
N2	0.0235 (15)	0.0214 (15)	0.0389 (19)	0.0056 (12)	0.0017 (13)	0.0009 (13)
N4	0.0273 (16)	0.0180 (14)	0.041 (2)	0.0069 (12)	−0.0018 (14)	0.0026 (13)
N3	0.0222 (16)	0.0287 (16)	0.037 (2)	0.0071 (13)	−0.0029 (13)	−0.0002 (14)
N5	0.0276 (16)	0.0180 (15)	0.041 (2)	0.0076 (12)	−0.0036 (14)	−0.0019 (13)
O1	0.0271 (13)	0.0215 (12)	0.0340 (15)	0.0065 (10)	−0.0060 (11)	−0.0003 (11)
O2	0.0399 (17)	0.0316 (15)	0.055 (2)	0.0174 (13)	−0.0175 (14)	0.0022 (14)
O3	0.0305 (15)	0.0226 (13)	0.0584 (19)	0.0087 (11)	−0.0122 (13)	0.0053 (13)
O4	0.0340 (16)	0.0369 (16)	0.0474 (18)	0.0156 (13)	−0.0170 (13)	−0.0050 (14)
O5	0.0457 (18)	0.0357 (16)	0.0323 (16)	0.0185 (13)	0.0007 (13)	0.0065 (13)
O6	0.147 (5)	0.045 (2)	0.069 (3)	0.048 (3)	−0.043 (3)	−0.004 (2)

Geometric parameters (Å, °)

Cu1—N1	1.974 (3)	C8—C9	1.353 (6)
Cu1—N4	2.056 (3)	C8—N2	1.369 (5)
Cu1—O5	2.076 (3)	C8—H8	0.9300
Cu1—N2	2.100 (3)	C9—N3	1.376 (5)
Cu1—O3	2.120 (3)	C9—H9	0.9300

Cu1—O1	2.141 (3)	C10—N2	1.321 (5)
C1—N1	1.330 (5)	C10—N3	1.331 (5)
C1—C2	1.378 (5)	C10—C11	1.449 (5)
C1—C6	1.525 (5)	C11—N4	1.324 (5)
C2—C3	1.384 (6)	C11—N5	1.341 (5)
C2—H2	0.9300	C12—C13	1.354 (6)
C3—C4	1.385 (6)	C12—N4	1.371 (5)
C3—H3	0.9300	C12—H12	0.9300
C4—C5	1.379 (5)	C13—N5	1.369 (6)
C4—H4	0.9300	C13—H13	0.9300
C5—N1	1.331 (5)	N3—H3A	0.83 (3)
C5—C7	1.529 (5)	N5—H5C	0.83 (3)
C6—O2	1.233 (5)	O5—H5A	0.80 (3)
C6—O1	1.267 (4)	O5—H5B	0.84 (3)
C7—O4	1.229 (5)	O6—H6A	0.84 (3)
C7—O3	1.270 (5)	O6—H6B	0.83 (3)
N1—Cu1—N4	173.29 (12)	N2—C8—H8	125.2
N1—Cu1—O5	95.10 (12)	C8—C9—N3	106.1 (4)
N4—Cu1—O5	91.07 (13)	C8—C9—H9	127.0
N1—Cu1—N2	94.58 (12)	N3—C9—H9	127.0
N4—Cu1—N2	79.94 (12)	N2—C10—N3	111.8 (3)
O5—Cu1—N2	164.58 (13)	N2—C10—C11	117.7 (3)
N1—Cu1—O3	77.85 (11)	N3—C10—C11	130.6 (3)
N4—Cu1—O3	99.15 (11)	N4—C11—N5	111.4 (3)
O5—Cu1—O3	93.90 (13)	N4—C11—C10	117.1 (3)
N2—Cu1—O3	99.86 (13)	N5—C11—C10	131.4 (4)
N1—Cu1—O1	77.50 (11)	C13—C12—N4	109.2 (4)
N4—Cu1—O1	105.69 (11)	C13—C12—H12	125.4
O5—Cu1—O1	85.31 (11)	N4—C12—H12	125.4
N2—Cu1—O1	85.10 (11)	C12—C13—N5	106.8 (3)
O3—Cu1—O1	155.16 (10)	C12—C13—H13	126.6
N1—C1—C2	120.4 (4)	N5—C13—H13	126.6
N1—C1—C6	112.9 (3)	C1—N1—C5	121.7 (3)
C2—C1—C6	126.6 (4)	C1—N1—Cu1	119.1 (2)
C1—C2—C3	118.3 (4)	C5—N1—Cu1	119.0 (2)
C1—C2—H2	120.8	C10—N2—C8	105.5 (3)
C3—C2—H2	120.8	C10—N2—Cu1	110.9 (2)
C2—C3—C4	120.8 (4)	C8—N2—Cu1	141.3 (3)
C2—C3—H3	119.6	C11—N4—C12	105.8 (3)
C4—C3—H3	119.6	C11—N4—Cu1	113.0 (2)
C5—C4—C3	117.4 (4)	C12—N4—Cu1	141.3 (3)
C5—C4—H4	121.3	C10—N3—C9	107.0 (3)
C3—C4—H4	121.3	C10—N3—H3A	127 (3)
N1—C5—C4	121.3 (3)	C9—N3—H3A	126 (3)
N1—C5—C7	112.9 (3)	C11—N5—C13	106.8 (3)
C4—C5—C7	125.7 (3)	C11—N5—H5C	127 (3)
O2—C6—O1	125.9 (4)	C13—N5—H5C	126 (3)
O2—C6—C1	119.3 (3)	C6—O1—Cu1	114.4 (2)
O1—C6—C1	114.7 (3)	C7—O3—Cu1	115.6 (2)

O4—C7—O3	126.3 (3)	Cu1—O5—H5A	116 (4)
O4—C7—C5	119.2 (3)	Cu1—O5—H5B	117 (4)
O3—C7—C5	114.4 (3)	H5A—O5—H5B	113 (4)
C9—C8—N2	109.7 (3)	H6A—O6—H6B	112 (5)
C9—C8—H8	125.2		
N1—C1—C2—C3	0.3 (6)	N4—Cu1—N2—C10	−10.2 (2)
C6—C1—C2—C3	177.6 (4)	O5—Cu1—N2—C10	44.9 (6)
C1—C2—C3—C4	−0.7 (7)	O3—Cu1—N2—C10	−107.9 (2)
C2—C3—C4—C5	0.7 (7)	O1—Cu1—N2—C10	96.7 (3)
C3—C4—C5—N1	−0.3 (6)	N1—Cu1—N2—C8	14.6 (4)
C3—C4—C5—C7	−179.4 (4)	N4—Cu1—N2—C8	−169.3 (4)
N1—C1—C6—O2	167.6 (3)	O5—Cu1—N2—C8	−114.1 (5)
C2—C1—C6—O2	−9.9 (6)	O3—Cu1—N2—C8	93.1 (4)
N1—C1—C6—O1	−8.0 (5)	O1—Cu1—N2—C8	−62.4 (4)
C2—C1—C6—O1	174.5 (4)	N5—C11—N4—C12	0.5 (4)
N1—C5—C7—O4	175.4 (4)	C10—C11—N4—C12	177.6 (3)
C4—C5—C7—O4	−5.4 (6)	N5—C11—N4—Cu1	−179.2 (2)
N1—C5—C7—O3	−3.9 (5)	C10—C11—N4—Cu1	−2.1 (4)
C4—C5—C7—O3	175.3 (4)	C13—C12—N4—C11	−0.9 (4)
N2—C8—C9—N3	0.4 (5)	C13—C12—N4—Cu1	178.6 (3)
N2—C10—C11—N4	−7.3 (5)	O5—Cu1—N4—C11	−160.8 (3)
N3—C10—C11—N4	172.6 (4)	N2—Cu1—N4—C11	6.6 (3)
N2—C10—C11—N5	169.0 (4)	O3—Cu1—N4—C11	105.0 (3)
N3—C10—C11—N5	−11.1 (7)	O1—Cu1—N4—C11	−75.4 (3)
N4—C12—C13—N5	1.0 (5)	O5—Cu1—N4—C12	19.6 (4)
C2—C1—N1—C5	0.0 (6)	N2—Cu1—N4—C12	−173.0 (4)
C6—C1—N1—C5	−177.6 (3)	O3—Cu1—N4—C12	−74.5 (4)
C2—C1—N1—Cu1	176.5 (3)	O1—Cu1—N4—C12	105.1 (4)
C6—C1—N1—Cu1	−1.1 (4)	N2—C10—N3—C9	1.2 (4)
C4—C5—N1—C1	−0.1 (6)	C11—C10—N3—C9	−178.7 (4)
C7—C5—N1—C1	179.1 (3)	C8—C9—N3—C10	−0.9 (4)
C4—C5—N1—Cu1	−176.5 (3)	N4—C11—N5—C13	0.1 (4)
C7—C5—N1—Cu1	2.6 (4)	C10—C11—N5—C13	−176.4 (4)
O5—Cu1—N1—C1	89.7 (3)	C12—C13—N5—C11	−0.6 (4)
N2—Cu1—N1—C1	−78.3 (3)	O2—C6—O1—Cu1	−162.8 (3)
O3—Cu1—N1—C1	−177.4 (3)	C1—C6—O1—Cu1	12.5 (4)
O1—Cu1—N1—C1	5.7 (3)	N1—Cu1—O1—C6	−10.3 (3)
O5—Cu1—N1—C5	−93.7 (3)	N4—Cu1—O1—C6	163.6 (3)
N2—Cu1—N1—C5	98.3 (3)	O5—Cu1—O1—C6	−106.6 (3)
O3—Cu1—N1—C5	−0.8 (3)	N2—Cu1—O1—C6	85.5 (3)
O1—Cu1—N1—C5	−177.8 (3)	O3—Cu1—O1—C6	−17.4 (4)
N3—C10—N2—C8	−0.9 (4)	O4—C7—O3—Cu1	−176.0 (3)
C11—C10—N2—C8	179.0 (3)	C5—C7—O3—Cu1	3.2 (4)
N3—C10—N2—Cu1	−167.5 (2)	N1—Cu1—O3—C7	−1.5 (3)
C11—C10—N2—Cu1	12.4 (4)	N4—Cu1—O3—C7	−175.4 (3)
C9—C8—N2—C10	0.3 (4)	O5—Cu1—O3—C7	92.9 (3)
C9—C8—N2—Cu1	160.1 (3)	N2—Cu1—O3—C7	−94.1 (3)
N1—Cu1—N2—C10	173.7 (3)	O1—Cu1—O3—C7	5.6 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O6—H6A···O3^{i}	0.84 (3)	1.90 (4)	2.700 (5)	160 (9)
O5—H5B···O6^{ii}	0.84 (3)	1.88 (3)	2.719 (5)	174 (5)
O5—H5A···O4^{iii}	0.80 (3)	2.01 (3)	2.813 (4)	175 (5)
N5—H5C···O2^{iv}	0.83 (3)	2.05 (3)	2.871 (5)	166 (4)
N3—H3A···O1^{iv}	0.83 (3)	1.97 (3)	2.729 (4)	152 (4)
C3—H3···O6	0.93	2.55	3.359 (6)	146
C13—H13···O2^{v}	0.93	2.43	3.298 (5)	156
C4—H4···O4^{vi}	0.93	2.48	3.294 (5)	147

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

Fig. 1

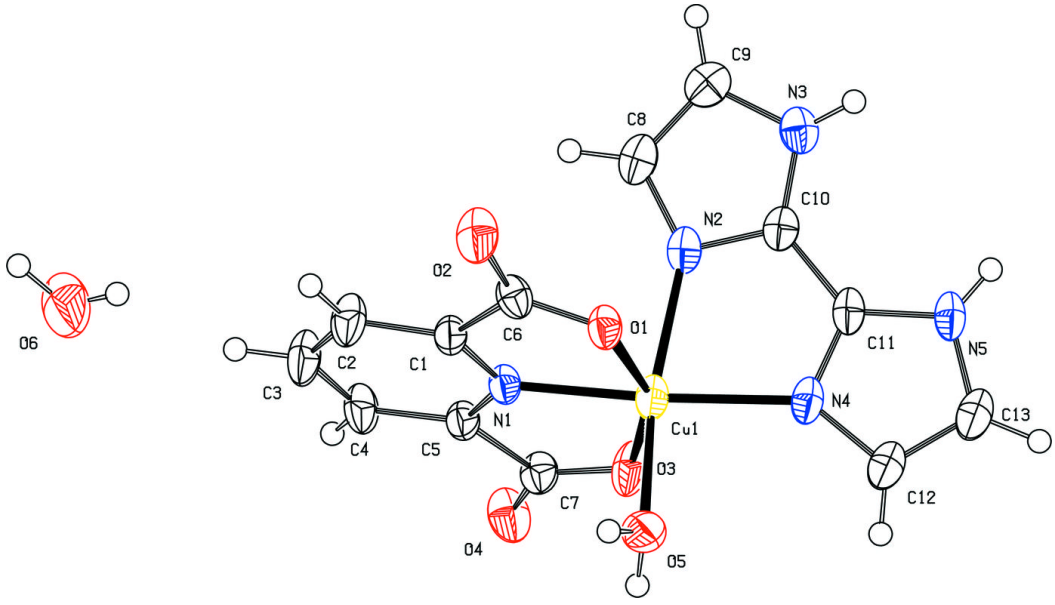
C9
N3
C8
C10
N2
O2
O1
C6
C11
N5
C2
C1
C3
N1
N4
C13
Cu1
C4
C5
O3
C7
C12
O4
O5
O6

Fig. 2