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Diaquabis[5-(pyrimidin-2-yl-κN)tetrazolato-κN^1]copper(II)

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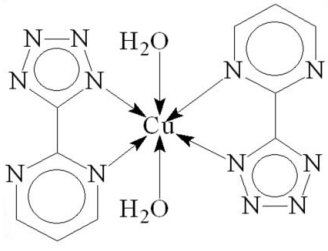
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.038; wR factor = 0.105; data-to-parameter ratio = 14.2.

The title compound, $[Cu(C_5H_3N_6)_2(H_2O)_2]$, is isostructural with the manganese(II) analogue, but different from the two-dimensional structures of the zinc(II), iron(II), cobalt(II) and nickel(II) complexes with the same 5-(pyrimidin-2-yl)tetrazolate ligand. Each of the two symmetry-independent but structurally similar mononuclear molecules in the crystallographic asymmetric unit occupies a special position with the Cu^{II} atom on an inversion centre. Both Cu^{II} atoms have a highly distorted octahedral coordination geometry formed by two *trans* water molecules and two chelating ligands. Intermolecular O—H···N hydrogen bonds are present, which lead to the formation of a two-dimensional network.

Related literature

For related literature, see: Liu & Fan (2007); Rodríguez *et al.* (2005, 2007); Rodríguez & Colacio (2006); Zhang *et al.* (2007).



Experimental

Crystal data

$[Cu(C_5H_3N_6)_2(H_2O)_2]$
M_r = 393.84
Triclinic, $P\overline{1}$
a = 7.329 (2) Å
b = 8.107 (2) Å
c = 12.926 (3) Å
α = 86.68 (3)°
β = 89.84 (3)°
γ = 77.49 (3)°
V = 748.5 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.50 mm^{-1}
T = 293 (2) K
0.40 × 0.30 × 0.28 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.956, T_{max} = 1.000
(expected range 0.629–0.658)
7532 measured reflections
3433 independent reflections
2314 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.105
S = 1.04
3433 reflections
241 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.66 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	1.977 (2)	Cu2—N7	1.967 (2)
Cu1—N5	2.057 (2)	Cu2—N11	2.062 (2)
Cu1—O1W	2.406 (2)	Cu2—O2W	2.411 (3)
N1—Cu1—N1^{i}	180	N7—Cu2—N7^{ii}	180
N1—Cu1—N5^{i}	99.14 (9)	N7—Cu2—N11	80.25 (10)
N1—Cu1—N5	80.86 (9)	N7^{ii}—Cu2—N11	99.75 (10)
N1—Cu1—O1W	89.66 (9)	N7—Cu2—O2W^{ii}	89.55 (9)
N1^{i}—Cu1—O1W	90.34 (9)	N7—Cu2—O2W	90.45 (9)
N5^{i}—Cu1—N5	180	N11—Cu2—O2W	92.58 (9)
N5^{i}—Cu1—O1W	89.00 (9)	N11—Cu2—O2W^{ii}	87.42 (9)
N5—Cu1—O1W	91.00 (9)	N11—Cu2—N11^{ii}	180
O1W^{i}—Cu1—O1W	180	O2W^{ii}—Cu2—O2W	180

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···N4^{iii}	0.84 (1)	2.11 (1)	2.939 (3)	169 (4)
O1W—H1WB···N10	0.84 (1)	2.03 (1)	2.869 (3)	174 (4)
O2W—H2WB···N3	0.85 (1)	2.02 (2)	2.845 (3)	164 (4)
O2W—H2WA···N9^{iv}	0.85 (1)	2.00 (1)	2.835 (3)	170 (4)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT* and *SHELXTL* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2417).

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supplementary materials

Acta Cryst. (2007). E**63**, m2718-m2719 [**doi:10.1107/S1600536807049197**]

Diaquabis[5-(pyrimidin-2-yl-κN)tetrazolato-κN^1]copper(II)

M.-F. Jin, Y.-E. Qiu and X.-L. Zhang

Comment

The crystal structures of Na^{II}, Mn^{II}, Fe^{II}, Co^{II}, Ni^{II} and Zn(II) complexes with 5-(pyrimidin-2-yl)tetrazolate group have been reported recently (Liu & Fan, 2007; Rodríguez *et al.*, 2005, 2007; Rodríguez & Colacio (2006); Zhang *et al.*, 2007). Such complexes were obtained by either the direction reaction of the ligand, 2-(1*H*-tetrazol-5-yl)pyrimidine or the *in situ* reaction from pyrimidine-2-carbonitrile in the presence of NaN_3 with metal salts under hydrothermal conditions. Except of the Mn^{II} complex, which has a mononuclear structure being similar to the title compound, all of other complexes have an extended structure, tow- or three-dimensional. And, the ligands coordinate to metal atoms adopting several modes.

The title complex, $Cu(C_5H_3N_6)_2(H_2O)_2$ (I) performs a mono-nuclear structure, being similar to that of Mn(II) analog. However, in the crystallographic asymmetric unit, there exist two symmetry-independent but structural similar mononuclear molecules, both of which occupies a special position with Cu^{II} atoms being on an inversion center (Fig. 1). Two Cu^{II} centers have a highly distorted octahedral coordination geometry formed by two *trans* water molecules and two chelating ligand moieties. Table 1 lists the related bond parameters. Furthermore, such molecules are assembled by the intermolecular O—H···N hydrogen bonds to form a two-dimensional network (Fig. 2 and Table 2).

Experimental

The title compound was synthesized as crystals by a hydrothermal method, with the ligand, 5-(pyrimidin-2-yl)tetrazolato formed during the reaction procedure from the pyrimidine-2-carbonitrile and NaN_3: A mixture of $CuCl_2{\cdot}2H_2O$ (17 mg, 0.1 mmol), NaN_3 (26 mg, 0.4 mmol) and pyrimidine-2-carbonitrile (21 mg, 0.2 mmol) in water (10 ml) was placed in a Teflon-lined stainless-steel Parr bomb that was heated at 443 K for 48 h. Blue crystals of (I) were collected after the bomb was allowed to cool to room temperature in the period of 24 h. Yield, 20% based on Cu^{II}. Caution: Azide and tetrazole derivatives are potentially explosive. Although we have met no problems in this work, only a small amount of them should be prepared and handled with great caution.

Refinement

H atoms of organic ligands were included in calculated positions and treated in the subsequent refinement as riding atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2 U_{eq}(C). The H atoms of water molecules were located in Fourier difference map and refined with bond restraints O—H = 0.85 (1) Å, and with U_{iso}(H) = 1.5 U_{eq} (O).

Figures

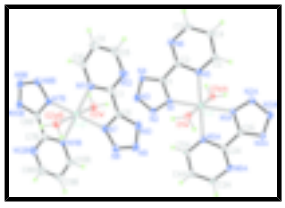

Fig. 1. Displacement ellipsoid plot (30% probability) of (I). [Symmetry codes: (A) −*x*, −*y*, 1 − *z*; (B) 1 − *x*, −*y*, −*z*]

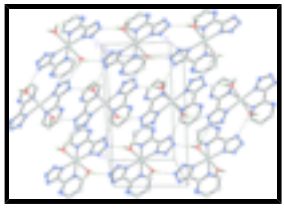

Fig. 2. Two-dimensional H-bonded network in (I).

Diaquabis[5-(pyrimidin-2-yl-κ*N*)tetrazolato-κN^1]copper(II)

Crystal data

$[Cu(C_5H_3N_6)_2(H_2O)_2]$	$Z = 2$
$M_r = 393.84$	$F_{000} = 398$
Triclinic, $P\overline{1}$	$D_x = 1.747$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.329$ (2) Å	Cell parameters from 5023 reflections
$b = 8.107$ (2) Å	$\theta = 3.1$–$27.5°$
$c = 12.926$ (3) Å	$\mu = 1.50$ mm^{-1}
$\alpha = 86.68$ (3)°	$T = 293$ (2) K
$\beta = 89.84$ (3)°	Block, blue
$\gamma = 77.49$ (3)°	0.40 × 0.30 × 0.28 mm
$V = 748.5$ (3) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	3433 independent reflections
Radiation source: fine-focus sealed tube	2314 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.043$
$T = 293(2)$ K	$\theta_{max} = 27.5°$
φ and ω scans	$\theta_{min} = 3.1°$
Absorption correction: multi-scan (SADABS; Bruker, 1998)	$h = -9 \rightarrow 9$
$T_{min} = 0.956$, $T_{max} = 1.000$	$k = -10 \rightarrow 10$
7532 measured reflections	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.038$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.105$	$w = 1/[\sigma^2(F_o^2) + (0.0465P)^2 + 0.1285P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$
3433 reflections	$\Delta\rho_{max} = 0.66$ e Å^{-3}
241 parameters	$\Delta\rho_{min} = -0.39$ e Å^{-3}
4 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 $F^2 > \sigma(F^2)$ 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	0.0000	0.0000	0.5000	0.02640 (15)
Cu2	0.5000	0.0000	0.0000	0.02917 (16)
N1	0.2252 (3)	−0.0382 (3)	0.41247 (18)	0.0262 (5)
N2	0.3163 (3)	−0.1505 (3)	0.3476 (2)	0.0314 (6)
N3	0.4635 (3)	−0.0956 (4)	0.3140 (2)	0.0341 (6)
N4	0.4700 (3)	0.0523 (3)	0.35479 (19)	0.0305 (6)
N5	0.1078 (3)	0.2025 (3)	0.53878 (18)	0.0253 (5)
N6	0.3470 (3)	0.3472 (3)	0.4879 (2)	0.0341 (6)
N7	0.2673 (3)	−0.0184 (3)	0.07146 (19)	0.0314 (6)
N8	0.1525 (4)	−0.1263 (4)	0.0808 (2)	0.0406 (7)
N9	0.0165 (4)	−0.0616 (4)	0.1429 (2)	0.0442 (8)
N10	0.0406 (3)	0.0868 (4)	0.1760 (2)	0.0389 (7)
N11	0.4647 (3)	0.2093 (3)	0.08732 (19)	0.0319 (6)
N12	0.2438 (4)	0.3698 (4)	0.1982 (2)	0.0470 (8)
C1	0.3220 (4)	0.0848 (4)	0.4138 (2)	0.0253 (6)
C2	0.2579 (4)	0.2218 (4)	0.4829 (2)	0.0252 (6)

C3	0.2810 (4)	0.4591 (4)	0.5590 (3)	0.0392 (8)
H3A	0.3380	0.5500	0.5653	0.047*
C4	0.1354 (4)	0.4464 (4)	0.6222 (3)	0.0367 (8)
H4A	0.0959	0.5240	0.6722	0.044*
C5	0.0488 (4)	0.3144 (4)	0.6093 (2)	0.0324 (7)
H5A	−0.0526	0.3034	0.6505	0.039*
C6	0.1972 (4)	0.1096 (4)	0.1310 (2)	0.0311 (7)
C7	0.3035 (4)	0.2396 (4)	0.1399 (2)	0.0327 (7)
C8	0.3586 (6)	0.4771 (5)	0.2042 (3)	0.0583 (11)
H8A	0.3225	0.5700	0.2443	0.070*
C9	0.5271 (6)	0.4569 (5)	0.1540 (3)	0.0535 (10)
H9A	0.6044	0.5330	0.1595	0.064*
C10	0.5751 (5)	0.3182 (4)	0.0952 (3)	0.0402 (8)
H10A	0.6880	0.3002	0.0601	0.048*
O1W	−0.1759 (3)	0.1664 (3)	0.35881 (17)	0.0339 (5)
H1WA	−0.279 (3)	0.139 (5)	0.349 (3)	0.051*
H1WB	−0.116 (4)	0.150 (5)	0.3033 (16)	0.051*
O2W	0.6811 (3)	−0.1811 (3)	0.13454 (17)	0.0390 (6)
H2WA	0.780 (3)	−0.146 (5)	0.145 (3)	0.059*
H2WB	0.631 (5)	−0.172 (5)	0.1934 (15)	0.059*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0222 (2)	0.0284 (3)	0.0324 (3)	−0.0114 (2)	0.0131 (2)	−0.0119 (2)
Cu2	0.0255 (3)	0.0347 (3)	0.0317 (3)	−0.0132 (2)	0.0132 (2)	−0.0133 (2)
N1	0.0231 (11)	0.0306 (14)	0.0267 (12)	−0.0076 (10)	0.0067 (10)	−0.0088 (11)
N2	0.0269 (12)	0.0342 (15)	0.0335 (14)	−0.0056 (11)	0.0080 (11)	−0.0093 (12)
N3	0.0247 (12)	0.0449 (17)	0.0318 (14)	−0.0045 (11)	0.0080 (11)	−0.0075 (13)
N4	0.0250 (12)	0.0383 (16)	0.0303 (14)	−0.0109 (11)	0.0072 (10)	−0.0029 (12)
N5	0.0229 (11)	0.0243 (13)	0.0299 (13)	−0.0075 (10)	0.0058 (10)	−0.0029 (11)
N6	0.0310 (13)	0.0355 (15)	0.0400 (15)	−0.0161 (11)	0.0054 (11)	−0.0043 (13)
N7	0.0255 (12)	0.0422 (16)	0.0277 (13)	−0.0093 (11)	0.0082 (11)	−0.0059 (12)
N8	0.0333 (14)	0.055 (2)	0.0373 (16)	−0.0170 (13)	0.0068 (12)	−0.0088 (14)
N9	0.0272 (13)	0.071 (2)	0.0380 (16)	−0.0179 (14)	0.0090 (12)	−0.0018 (16)
N10	0.0289 (13)	0.055 (2)	0.0331 (15)	−0.0086 (13)	0.0107 (11)	−0.0049 (14)
N11	0.0317 (13)	0.0349 (15)	0.0307 (14)	−0.0089 (11)	0.0065 (11)	−0.0082 (12)
N12	0.0540 (18)	0.0377 (18)	0.0479 (18)	−0.0039 (14)	0.0142 (15)	−0.0146 (15)
C1	0.0216 (13)	0.0310 (16)	0.0246 (14)	−0.0092 (12)	0.0035 (11)	−0.0003 (12)
C2	0.0207 (12)	0.0277 (15)	0.0287 (15)	−0.0086 (11)	0.0021 (11)	−0.0006 (12)
C3	0.0395 (17)	0.0319 (18)	0.052 (2)	−0.0191 (14)	0.0014 (16)	−0.0077 (16)
C4	0.0395 (17)	0.0320 (18)	0.0411 (19)	−0.0107 (14)	0.0060 (15)	−0.0124 (15)
C5	0.0320 (15)	0.0313 (17)	0.0364 (17)	−0.0097 (13)	0.0092 (13)	−0.0126 (15)
C6	0.0247 (14)	0.0409 (19)	0.0256 (15)	−0.0027 (13)	0.0055 (12)	−0.0003 (14)
C7	0.0345 (16)	0.0343 (18)	0.0265 (15)	−0.0013 (13)	0.0031 (13)	−0.0022 (14)
C8	0.077 (3)	0.038 (2)	0.058 (3)	−0.006 (2)	0.014 (2)	−0.022 (2)
C9	0.069 (3)	0.042 (2)	0.056 (2)	−0.0211 (19)	0.006 (2)	−0.0161 (19)
C10	0.0427 (18)	0.039 (2)	0.0428 (19)	−0.0169 (16)	0.0047 (15)	−0.0087 (16)

O1W	0.0297 (11)	0.0397 (13)	0.0347 (13)	−0.0116 (10)	0.0073 (10)	−0.0071 (11)
O2W	0.0337 (12)	0.0525 (15)	0.0354 (13)	−0.0177 (11)	0.0086 (10)	−0.0097 (12)

Geometric parameters (Å, °)

Cu1—N1	1.977 (2)	N8—N9	1.316 (4)
Cu1—N5	2.057 (2)	N9—N10	1.347 (4)
Cu1—O1W	2.406 (2)	N10—C6	1.328 (4)
Cu2—N7	1.967 (2)	N11—C10	1.328 (4)
Cu2—N11	2.062 (2)	N11—C7	1.345 (4)
Cu2—O2W	2.411 (3)	N12—C7	1.329 (4)
Cu1—N1^{i}	1.977 (2)	N12—C8	1.340 (5)
Cu1—N5^{i}	2.057 (2)	C1—C2	1.463 (4)
Cu1—O1W^{i}	2.406 (2)	C3—C4	1.360 (4)
Cu2—N7^{ii}	1.967 (2)	C3—H3A	0.9300
Cu2—N11^{ii}	2.062 (2)	C4—C5	1.375 (4)
Cu2—O2W^{ii}	2.411 (3)	C4—H4A	0.9300
N1—N2	1.342 (3)	C5—H5A	0.9300
N1—C1	1.344 (4)	C6—C7	1.449 (4)
N2—N3	1.317 (3)	C8—C9	1.376 (5)
N3—N4	1.348 (3)	C8—H8A	0.9300
N4—C1	1.313 (3)	C9—C10	1.375 (4)
N5—C5	1.328 (3)	C9—H9A	0.9300
N5—C2	1.346 (3)	C10—H10A	0.9300
N6—C2	1.326 (4)	O1W—H1WA	0.842 (10)
N6—C3	1.343 (4)	O1W—H1WB	0.841 (10)
N7—N8	1.339 (4)	O2W—H2WA	0.847 (10)
N7—C6	1.339 (4)	O2W—H2WB	0.845 (10)
N1—Cu1—N1^{i}	180.0	N9—N8—N7	107.5 (3)
N1—Cu1—N5^{i}	99.14 (9)	N8—N9—N10	110.7 (3)
N1—Cu1—N5	80.86 (9)	C6—N10—N9	104.5 (3)
N1—Cu1—O1W	89.66 (9)	C10—N11—C7	117.2 (3)
N1^{i}—Cu1—O1W	90.34 (9)	C10—N11—Cu2	129.0 (2)
N5^{i}—Cu1—N5	180.00 (6)	C7—N11—Cu2	113.8 (2)
N5^{i}—Cu1—O1W	89.00 (9)	C7—N12—C8	115.4 (3)
N5—Cu1—O1W	91.00 (9)	N4—C1—N1	111.4 (3)
O1W^{i}—Cu1—O1W	180.00 (7)	N4—C1—C2	130.8 (3)
N1^{i}—Cu1—N5^{i}	80.86 (9)	N1—C1—C2	117.7 (2)
N1^{i}—Cu1—N5	99.14 (9)	N6—C2—N5	126.1 (3)
N1—Cu1—O1W^{i}	90.34 (9)	N6—C2—C1	120.7 (3)
N1^{i}—Cu1—O1W^{i}	89.66 (9)	N5—C2—C1	113.1 (2)
N5^{i}—Cu1—O1W^{i}	91.00 (9)	N6—C3—C4	123.5 (3)
N5—Cu1—O1W^{i}	89.00 (9)	N6—C3—H3A	118.3
N7—Cu2—N7^{ii}	180.0 (2)	C4—C3—H3A	118.3
N7—Cu2—N11	80.25 (10)	C3—C4—C5	117.4 (3)

N7^{ii}—Cu2—N11	99.75 (10)	C3—C4—H4A	121.3
N7—Cu2—O2W^{ii}	89.55 (9)	C5—C4—H4A	121.3
N7—Cu2—O2W	90.45 (9)	N5—C5—C4	121.0 (3)
N11—Cu2—O2W	92.58 (9)	N5—C5—H5A	119.5
N11—Cu2—O2W^{ii}	87.42 (9)	C4—C5—H5A	119.5
N11—Cu2—N11^{ii}	180.00 (12)	N10—C6—N7	110.8 (3)
O2W^{ii}—Cu2—O2W	180.00 (19)	N10—C6—C7	131.7 (3)
N7—Cu2—N11^{ii}	99.75 (10)	N7—C6—C7	117.4 (3)
N7^{ii}—Cu2—N11^{ii}	80.25 (10)	N12—C7—N11	125.8 (3)
N7^{ii}—Cu2—O2W^{ii}	90.45 (9)	N12—C7—C6	121.0 (3)
N11^{ii}—Cu2—O2W^{ii}	92.58 (9)	N11—C7—C6	113.2 (3)
N7^{ii}—Cu2—O2W	89.55 (9)	N12—C8—C9	123.4 (3)
N11^{ii}—Cu2—O2W	87.42 (9)	N12—C8—H8A	118.3
N2—N1—C1	105.9 (2)	C9—C8—H8A	118.3
N2—N1—Cu1	140.0 (2)	C10—C9—C8	116.5 (3)
C1—N1—Cu1	114.09 (18)	C10—C9—H9A	121.7
N3—N2—N1	107.4 (2)	C8—C9—H9A	121.7
N2—N3—N4	110.7 (2)	N11—C10—C9	121.8 (3)
C1—N4—N3	104.6 (2)	N11—C10—H10A	119.1
C5—N5—C2	117.2 (2)	C9—C10—H10A	119.1
C5—N5—Cu1	129.0 (2)	Cu1—O1W—H1WA	112 (3)
C2—N5—Cu1	113.81 (18)	Cu1—O1W—H1WB	110 (3)
C2—N6—C3	114.8 (3)	H1WA—O1W—H1WB	106 (3)
N8—N7—C6	106.5 (2)	Cu2—O2W—H2WA	109 (3)
N8—N7—Cu2	138.6 (2)	Cu2—O2W—H2WB	113 (3)
C6—N7—Cu2	114.9 (2)	H2WA—O2W—H2WB	102 (4)
N5^{i}—Cu1—N1—N2	−3.7 (3)	N2—N1—C1—N4	−1.3 (3)
N5—Cu1—N1—N2	176.3 (3)	Cu1—N1—C1—N4	179.71 (19)
O1W^{i}—Cu1—N1—N2	87.4 (3)	N2—N1—C1—C2	−177.1 (2)
O1W—Cu1—N1—N2	−92.6 (3)	Cu1—N1—C1—C2	3.9 (3)
N5^{i}—Cu1—N1—C1	174.8 (2)	C3—N6—C2—N5	2.6 (5)
N5—Cu1—N1—C1	−5.2 (2)	C3—N6—C2—C1	−176.1 (3)
O1W^{i}—Cu1—N1—C1	−94.1 (2)	C5—N5—C2—N6	−3.7 (5)
O1W—Cu1—N1—C1	85.9 (2)	Cu1—N5—C2—N6	175.8 (2)
C1—N1—N2—N3	1.1 (3)	C5—N5—C2—C1	175.1 (3)
Cu1—N1—N2—N3	179.7 (2)	Cu1—N5—C2—C1	−5.5 (3)
N1—N2—N3—N4	−0.6 (3)	N4—C1—C2—N6	5.2 (5)
N2—N3—N4—C1	−0.1 (3)	N1—C1—C2—N6	−179.9 (3)
N1^{i}—Cu1—N5—C5	5.3 (3)	N4—C1—C2—N5	−173.7 (3)
O1W^{i}—Cu1—N5—C5	−84.2 (3)	N1—C1—C2—N5	1.2 (4)
O1W—Cu1—N5—C5	95.8 (3)	C2—N6—C3—C4	0.5 (5)
N1—Cu1—N5—C2	6.0 (2)	N6—C3—C4—C5	−2.2 (5)
N1^{i}—Cu1—N5—C2	−174.0 (2)	C2—N5—C5—C4	1.6 (4)
O1W^{i}—Cu1—N5—C2	96.5 (2)	Cu1—N5—C5—C4	−177.7 (2)
O1W—Cu1—N5—C2	−83.5 (2)	C3—C4—C5—N5	1.1 (5)

N11—Cu2—N7—N8	−174.2 (3)	N9—N10—C6—N7	0.6 (4)
N11^{ii}—Cu2—N7—N8	5.8 (3)	N9—N10—C6—C7	−175.9 (3)
O2W^{ii}—Cu2—N7—N8	98.3 (3)	N8—N7—C6—N10	−1.0 (4)
O2W—Cu2—N7—N8	−81.7 (3)	Cu2—N7—C6—N10	179.9 (2)
N11—Cu2—N7—C6	4.4 (2)	N8—N7—C6—C7	176.0 (3)
N11^{ii}—Cu2—N7—C6	−175.6 (2)	Cu2—N7—C6—C7	−3.0 (4)
O2W^{ii}—Cu2—N7—C6	−83.0 (2)	C8—N12—C7—N11	−0.7 (5)
O2W—Cu2—N7—C6	97.0 (2)	C8—N12—C7—C6	176.9 (3)
C6—N7—N8—N9	1.1 (4)	C10—N11—C7—N12	0.8 (5)
Cu2—N7—N8—N9	179.8 (2)	Cu2—N11—C7—N12	−177.1 (3)
N7—N8—N9—N10	−0.7 (4)	C10—N11—C7—C6	−176.9 (3)
N8—N9—N10—C6	0.1 (4)	Cu2—N11—C7—C6	5.2 (3)
N7—Cu2—N11—C10	177.1 (3)	N10—C6—C7—N12	−3.1 (6)
N7^{ii}—Cu2—N11—C10	−2.9 (3)	N7—C6—C7—N12	−179.5 (3)
O2W^{ii}—Cu2—N11—C10	−92.9 (3)	N10—C6—C7—N11	174.7 (3)
O2W—Cu2—N11—C10	87.1 (3)	N7—C6—C7—N11	−1.6 (4)
N7—Cu2—N11—C7	−5.4 (2)	C7—N12—C8—C9	0.2 (6)
N7^{ii}—Cu2—N11—C7	174.6 (2)	N12—C8—C9—C10	0.2 (6)
O2W^{ii}—Cu2—N11—C7	84.6 (2)	C7—N11—C10—C9	−0.4 (5)
O2W—Cu2—N11—C7	−95.4 (2)	Cu2—N11—C10—C9	177.1 (3)
N3—N4—C1—N1	0.9 (3)	C8—C9—C10—N11	0.0 (6)
N3—N4—C1—C2	176.0 (3)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1WA···N4^{iii}	0.84 (1)	2.11 (1)	2.939 (3)	169 (4)
O1W—H1WB···N10	0.84 (1)	2.03 (1)	2.869 (3)	174 (4)
O2W—H2WB···N3	0.85 (1)	2.02 (2)	2.845 (3)	164 (4)
O2W—H2WA···N9^{iv}	0.85 (1)	2.00 (1)	2.835 (3)	170 (4)

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

Fig. 1

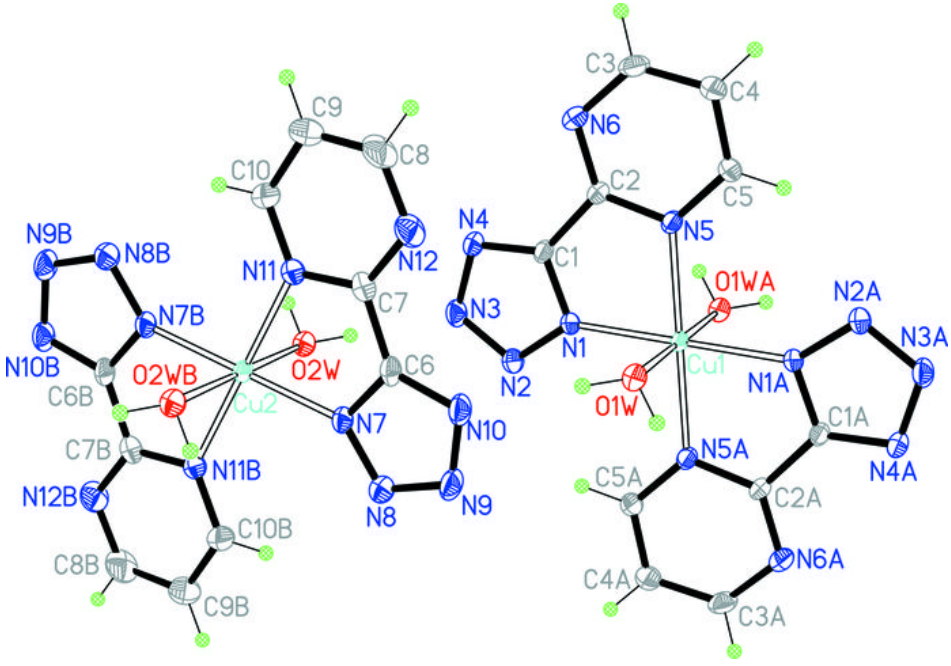
C3
C4
N6
C2
C5
N5
C9
C8
C10
N4
C1
O1WA
N2A
N3A
N9B
N8B
N11
N12
C7
N3
N1
Cu1
N1A
N7B
O2W
C6
N10B
O2WB
Cu2
N2
O1W
C6B
N7
N10
C1A
N4A
C7B
N11B
N5A
C5A
N12B
N8
N9
C2A
C10B
N6A
C8B
C4A
C9B
C3A

Fig. 2