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Poly[diaquabis{μ-5-[4-(1*H*-imidazol-1-ylmethyl)phenyl]tetrazolato}copper(II)]

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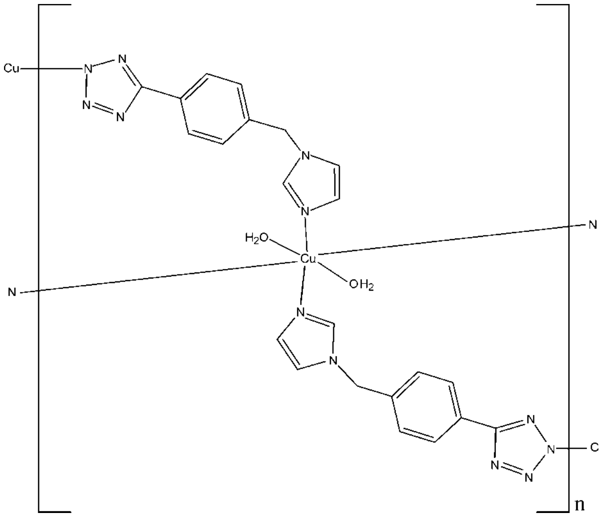
Key indicators: single-crystal X-ray study; *T* = 293 K; mean σ(C–C) = 0.003 Å; *R* factor = 0.031; *wR* factor = 0.085; data-to-parameter ratio = 12.7.

In the title compound, $[Cu(C_{11}H_9N_6)_2(H_2O)_2]_n$, the Cu^{II} atom lies on an inversion center and is coordinated by four N atoms from four 5-[4-(1*H*-imidazol-1-ylmethyl)phenyl]tetrazolate ligands and two water molecules in a distorted octahedral geometry. The ligands bridge the Cu^{II} atoms, leading to the formation of a two-dimensional network parallel to (100). The structure is further stabilized by O—H···N hydrogen bonds within the network.

Related literature

For background to metal-organic architectures, see: Song *et al.* (2012); Wang *et al.* (2010). For background to metal-azolate frameworks, see: Masciocchi *et al.* (2005). For a related structure, see: Zhang *et al.* (2006).



Experimental

Crystal data

$[Cu(C_{11}H_9N_6)_2(H_2O)_2]$
M_r = 550.06
Monoclinic, $P2_1/c$
a = 7.3363 (10) Å
b = 6.1934 (9) Å
c = 25.219 (4) Å
β = 97.708 (2)°
V = 1135.5 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.01 mm^{-1}
T = 293 K
0.25 × 0.21 × 0.20 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.751, T_{max} = 0.824
6050 measured reflections
2224 independent reflections
2064 reflections with $I > 2\sigma(I)$
R_{int} = 0.015

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.085
S = 1.09
2224 reflections
175 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—N1	2.0247 (15)	Cu1—O1*W*	2.610 (2)
Cu1—N6^i	1.9909 (16)		

Symmetry code: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*A*···N3^{ii}	0.90 (2)	2.07 (2)	2.929 (3)	161 (3)

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *XP* in *SHELXTL* and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL*.

We thank Changchun Normal University for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2532).

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supplementary materials

Acta Cryst. (2012). E**68**, m622 [doi:10.1107/S1600536812015176]

Poly[diaquabis{*μ*-5-[4-(1*H*-imidazol-1-ylmethyl)phenyl]tetrazolato}copper(II)]

Yuan Li and Ruizhan Chen

Comment

Metal-organic architectures constructed by flexible, multifunctional ligands often exhibit structural diversity (Song *et al.*, 2012; Wang *et al.*, 2010). Metal-azolate frameworks, being composed of transition metal ions and deprotonated five-membered heterocycles, are regarded as a great achievement in understanding supramolecular isomerism (Masciocchi *et al.*, 2005). The azolate nitrogen donors can be presicely controlled as coordination and guest binding sites. In addition to the strong coordination ability toward transition metal ions, azolate ligands also combine the negative charge of carboxylates and predictable coordination modes of pyridines. Recently, we obtained the title complex by the reaction of copper chloride with 5-(4-imidazol-1-yl-benzyl)-2*H*-tetrazole using hydrothermal method and its crystal structure is reported here.

In the title compound, the Cu^{II} atom lies on an inversion center and adopts a distorted octahedral coordination geometry, being coordinated by four N atoms from four azolate ligands and two water molecules (Fig. 1, Table 1). The Cu—O and Cu—N bond lengths and the bond angles are in the normal range (Zhang *et al.*, 2006). The bridging azolate ligands allow the formation of a two-dimensional network parallel to (1 0 0) (Fig. 2). The crystal structure is further stabilized by O—H···N hydrogen bonds within the network (Table 2).

Experimental

A mixture of $CuCl_2.2H_2O$ (0.2 mmol, 0.034 g), 5-(4-imidazol-1-yl-benzyl)-2*H*-tetrazole (0.2 mmol, 0.045 g), NaOH (0.2 mmol, 0.008 g) and water (10 ml) was sealed in a 15 ml Teflon-lined reactor, which was heated at 120°C for 72 h and then gradually cooled to room temperature. Blue crystals were obtained.

Refinement

H atoms on C atoms were generated geometrically and refined as riding atoms, with C—H = 0.93 (aromatic) and 0.97 (CH_2) Å and $U_{iso}(H) = 1.2U_{eq}(C)$. Water H atoms were located in a difference Fourier map and refined with $U_{iso}(H) = 1.5U_{eq}(O)$.

Computing details

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

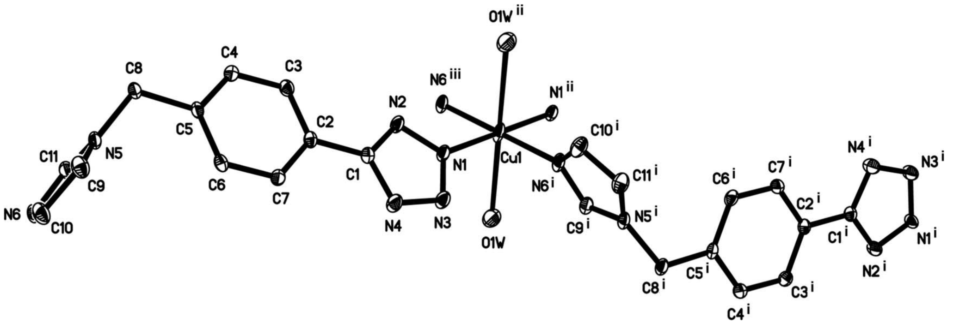

Figure 1

The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry codes: (i) x, 1/2-y, 1/2+z; (ii) -x, -y, 1-z; (iii) -x, -1/2+y, 1/2-z.]

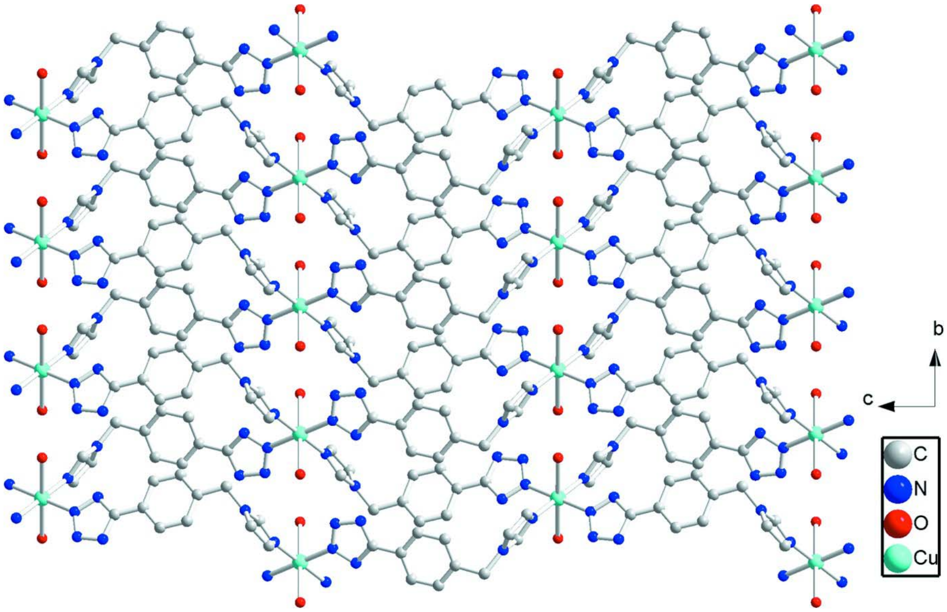

Figure 2

View of the two-dimensional network.

Poly[diaquabis{*μ*-5-[4-(1*H*-imidazol-1- ylmethyl)phenyl]tetrazolato}copper(II)]

Crystal data

$[Cu(C_{11}H_9N_6)_2(H_2O)_2]$
$M_r = 550.06$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.3363$ (10) Å
$b = 6.1934$ (9) Å
$c = 25.219$ (4) Å
$\beta = 97.708$ (2)°
$V = 1135.5$ (3) Å^3
$Z = 2$

$F(000) = 566$
$D_x = 1.609$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2224 reflections
$\theta = 1.0$–26.0°
$\mu = 1.01$ mm^{-1}
$T = 293$ K
Block, blue
0.25 × 0.21 × 0.20 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{\min} = 0.751$, $T_{\max} = 0.824$

6050 measured reflections
2224 independent reflections
2064 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.015$
$\theta_{\max} = 26.0°$, $\theta_{\min} = 1.6°$
$h = -6\rightarrow9$
$k = -7\rightarrow7$
$l = -27\rightarrow31$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.085$
$S = 1.09$
2224 reflections
175 parameters
2 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.044P)^2 + 0.7185P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.35$ e Å^{-3}
$\Delta\rho_{\min} = -0.29$ 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.

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	0.03061 (14)
C1	0.1942 (2)	0.1287 (3)	0.35950 (7)	0.0210 (4)
C2	0.2239 (2)	0.0738 (3)	0.30431 (7)	0.0206 (4)
C3	0.1855 (3)	−0.1330 (3)	0.28390 (7)	0.0238 (4)
H3	0.1428	−0.2387	0.3054	0.029*
C4	0.2110 (3)	−0.1813 (3)	0.23170 (7)	0.0241 (4)
H4	0.1839	−0.3193	0.2183	0.029*
C5	0.2764 (2)	−0.0262 (3)	0.19905 (7)	0.0204 (4)
C6	0.3139 (3)	0.1795 (3)	0.21932 (7)	0.0246 (4)
H6	0.3571	0.2848	0.1978	0.030*
C7	0.2875 (3)	0.2295 (3)	0.27156 (7)	0.0235 (4)
H7	0.3126	0.3682	0.2847	0.028*
C8	0.3083 (3)	−0.0898 (3)	0.14277 (7)	0.0252 (4)
H8A	0.4269	−0.1604	0.1444	0.030*
H8B	0.2147	−0.1928	0.1285	0.030*
C9	0.1502 (3)	0.1771 (3)	0.07892 (7)	0.0252 (4)

H9	0.0324	0.1233	0.0800	0.030*
C10	0.3754 (3)	0.3717 (4)	0.06022 (8)	0.0337 (5)
H10	0.4416	0.4790	0.0454	0.040*
C11	0.4493 (3)	0.2182 (4)	0.09521 (8)	0.0315 (5)
H11	0.5727	0.2005	0.1087	0.038*
N1	0.1185 (2)	0.1067 (3)	0.43685 (6)	0.0249 (3)
N2	0.1231 (3)	−0.0072 (2)	0.39174 (7)	0.0287 (4)
N3	0.1844 (2)	0.3016 (3)	0.43178 (6)	0.0293 (4)
N4	0.2332 (3)	0.3209 (3)	0.38258 (7)	0.0316 (4)
N5	0.3034 (2)	0.0945 (3)	0.10656 (6)	0.0230 (3)
N6	0.1884 (2)	0.3443 (3)	0.05002 (6)	0.0273 (4)
O1W	−0.2368 (3)	0.3145 (3)	0.50004 (7)	0.0427 (4)
H1A	−0.214 (4)	0.447 (3)	0.5139 (12)	0.064*
H1B	−0.336 (3)	0.265 (5)	0.5113 (12)	0.064*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0456 (2)	0.0346 (2)	0.01278 (19)	−0.02094 (15)	0.00818 (14)	−0.00562 (13)
C1	0.0209 (9)	0.0248 (9)	0.0174 (9)	−0.0010 (7)	0.0029 (7)	−0.0002 (7)
C2	0.0200 (8)	0.0262 (9)	0.0160 (9)	0.0007 (7)	0.0041 (6)	0.0006 (7)
C3	0.0276 (9)	0.0250 (10)	0.0195 (9)	−0.0025 (8)	0.0062 (7)	0.0033 (7)
C4	0.0296 (10)	0.0230 (9)	0.0198 (9)	−0.0006 (8)	0.0036 (7)	−0.0006 (7)
C5	0.0206 (9)	0.0264 (9)	0.0139 (9)	0.0048 (7)	0.0012 (7)	0.0025 (7)
C6	0.0308 (10)	0.0270 (10)	0.0170 (9)	−0.0009 (8)	0.0067 (7)	0.0058 (7)
C7	0.0289 (10)	0.0227 (9)	0.0188 (9)	−0.0029 (8)	0.0034 (7)	−0.0007 (7)
C8	0.0345 (10)	0.0261 (10)	0.0153 (9)	0.0079 (8)	0.0043 (7)	0.0033 (7)
C9	0.0283 (10)	0.0286 (10)	0.0185 (9)	0.0068 (8)	0.0030 (7)	0.0025 (7)
C10	0.0367 (11)	0.0403 (12)	0.0265 (11)	0.0037 (9)	0.0136 (9)	0.0104 (9)
C11	0.0276 (10)	0.0408 (12)	0.0271 (10)	0.0025 (9)	0.0070 (8)	0.0062 (9)
N1	0.0346 (9)	0.0250 (8)	0.0160 (7)	−0.0079 (7)	0.0064 (6)	−0.0040 (6)
N2	0.0454 (11)	0.0258 (9)	0.0167 (8)	−0.0091 (7)	0.0110 (7)	−0.0039 (6)
N3	0.0429 (10)	0.0269 (9)	0.0200 (8)	−0.0103 (7)	0.0116 (7)	−0.0042 (6)
N4	0.0479 (11)	0.0281 (9)	0.0217 (8)	−0.0110 (8)	0.0149 (7)	−0.0035 (7)
N5	0.0276 (8)	0.0282 (8)	0.0134 (7)	0.0056 (7)	0.0039 (6)	0.0024 (6)
N6	0.0362 (9)	0.0324 (9)	0.0142 (7)	0.0107 (7)	0.0067 (6)	0.0041 (6)
O1W	0.0577 (11)	0.0355 (9)	0.0361 (9)	−0.0071 (8)	0.0100 (8)	−0.0050 (7)

Geometric parameters (Å, º)

Cu1—N1	2.0247 (15)	C8—N5	1.459 (2)
Cu1—N6^{i}	1.9909 (16)	C8—H8A	0.9700
Cu1—O1W	2.610 (2)	C8—H8B	0.9700
C1—N2	1.325 (2)	C9—N6	1.318 (3)
C1—N4	1.339 (2)	C9—N5	1.341 (2)
C1—C2	1.477 (2)	C9—H9	0.9300
C2—C7	1.391 (3)	C10—C11	1.359 (3)
C2—C3	1.395 (3)	C10—N6	1.372 (3)
C3—C4	1.387 (3)	C10—H10	0.9300
C3—H3	0.9300	C11—N5	1.378 (3)

C4—C5	1.392 (3)	C11—H11	0.9300
C4—H4	0.9300	N1—N3	1.313 (2)
C5—C6	1.386 (3)	N1—N2	1.343 (2)
C5—C8	1.521 (2)	N3—N4	1.342 (2)
C6—C7	1.392 (3)	O1W—H1A	0.900 (18)
C6—H6	0.9300	O1W—H1B	0.874 (18)
C7—H7	0.9300		

N6$^{\text{ii}}$—Cu1—N6$^{\text{i}}$	180.00	C2—C7—H7	119.7
N6$^{\text{ii}}$—Cu1—N1	89.67 (6)	C6—C7—H7	119.7
N6$^{\text{i}}$—Cu1—N1	90.33 (6)	N5—C8—C5	112.80 (15)
N6$^{\text{ii}}$—Cu1—N1$^{\text{iii}}$	90.33 (6)	N5—C8—H8A	109.0
N6$^{\text{i}}$—Cu1—N1$^{\text{iii}}$	89.67 (6)	C5—C8—H8A	109.0
N1—Cu1—N1$^{\text{iii}}$	180.0	N5—C8—H8B	109.0
O1W—Cu1—N1	96.47 (6)	C5—C8—H8B	109.0
O1W—Cu1—N6$^{\text{ii}}$	87.49 (7)	H8A—C8—H8B	107.8
O1W—Cu1—O1W$^{\text{iii}}$	180.00	N6—C9—N5	111.21 (18)
O1W—Cu1—N1$^{\text{iii}}$	83.53 (6)	N6—C9—H9	124.4
O1W—Cu1—N6$^{\text{i}}$	92.51 (7)	N5—C9—H9	124.4
N2—C1—N4	112.13 (16)	C11—C10—N6	109.69 (18)
N2—C1—C2	123.50 (16)	C11—C10—H10	125.2
N4—C1—C2	124.37 (16)	N6—C10—H10	125.2
C7—C2—C3	119.01 (16)	C10—C11—N5	105.68 (18)
C7—C2—C1	120.23 (17)	C10—C11—H11	127.2
C3—C2—C1	120.75 (16)	N5—C11—H11	127.2
C4—C3—C2	120.16 (17)	N3—N1—N2	110.41 (15)
C4—C3—H3	119.9	N3—N1—Cu1	125.39 (12)
C2—C3—H3	119.9	N2—N1—Cu1	123.89 (12)
C3—C4—C5	120.89 (17)	C1—N2—N1	104.08 (15)
C3—C4—H4	119.6	N1—N3—N4	108.63 (15)
C5—C4—H4	119.6	C1—N4—N3	104.76 (15)
C6—C5—C4	118.91 (16)	C9—N5—C11	107.46 (16)
C6—C5—C8	122.29 (16)	C9—N5—C8	124.89 (16)
C4—C5—C8	118.79 (16)	C11—N5—C8	127.63 (16)
C5—C6—C7	120.50 (17)	C9—N6—C10	105.94 (16)
C5—C6—H6	119.8	C9—N6—Cu1$^{\text{iv}}$	123.39 (14)
C7—C6—H6	119.8	C10—N6—Cu1$^{\text{iv}}$	130.58 (14)
C2—C7—C6	120.53 (17)	H1A—O1W—H1B	109 (3)

N2—C1—C2—C7	175.61 (18)	N6$^{\text{i}}$—Cu1—N1—N2	146.67 (17)
N4—C1—C2—C7	−3.5 (3)	N4—C1—N2—N1	−0.1 (2)
N2—C1—C2—C3	−3.2 (3)	C2—C1—N2—N1	−179.28 (17)
N4—C1—C2—C3	177.71 (18)	N3—N1—N2—C1	−0.2 (2)
C7—C2—C3—C4	0.0 (3)	Cu1—N1—N2—C1	173.62 (13)
C1—C2—C3—C4	178.88 (17)	N2—N1—N3—N4	0.4 (2)
C2—C3—C4—C5	0.6 (3)	Cu1—N1—N3—N4	−173.29 (13)
C3—C4—C5—C6	−0.8 (3)	N2—C1—N4—N3	0.3 (2)
C3—C4—C5—C8	177.86 (17)	C2—C1—N4—N3	179.51 (17)
C4—C5—C6—C7	0.3 (3)	N1—N3—N4—C1	−0.4 (2)

C8—C5—C6—C7	−178.27 (17)	N6—C9—N5—C11	0.8 (2)
C3—C2—C7—C6	−0.5 (3)	N6—C9—N5—C8	179.32 (16)
C1—C2—C7—C6	−179.34 (17)	C10—C11—N5—C9	−0.5 (2)
C5—C6—C7—C2	0.3 (3)	C10—C11—N5—C8	−178.94 (17)
C6—C5—C8—N5	−24.7 (3)	C5—C8—N5—C9	−85.6 (2)
C4—C5—C8—N5	156.69 (17)	C5—C8—N5—C11	92.7 (2)
N6—C10—C11—N5	0.0 (2)	N5—C9—N6—C10	−0.8 (2)
N6^{ii}—Cu1—N1—N3	139.55 (17)	N5—C9—N6—Cu1^{iv}	176.09 (12)
N6^{i}—Cu1—N1—N3	−40.45 (17)	C11—C10—N6—C9	0.5 (2)
N6^{ii}—Cu1—N1—N2	−33.33 (17)	C11—C10—N6—Cu1^{iv}	−176.08 (14)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*A*···N3^{v}	0.90 (2)	2.07 (2)	2.929 (3)	161 (3)

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