Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diaquabis[5-(2-pyrazin-2-yl)tetrazolato]-copper(II)–pyrazine-2-carbonitrile (1/2)

Mohamed Abdellatif Bensegueni,[a]* Aouatef Cherouana,[a] Slimane Dahaoui[b] and Issam Boudraa[a]

[a]Unité de Recherche de Chimie de l'Environnement et Moléculaire Structurale, Université Constantine 1, Algeria, and [b]CRM2, UMR-CNRS 7036, Jean Barriol Institut, Lorraine University, BP 230, 54506 Vandoeuvre-lés-Nancy Cedex, France
Correspondence e-mail: bm_abdel@yahoo.fr

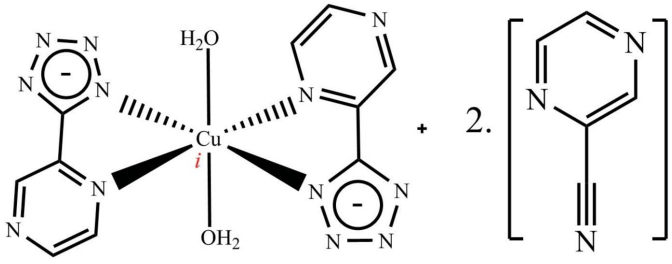
Received 30 November 2013; accepted 30 January 2014

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.027; wR factor = 0.075; data-to-parameter ratio = 19.0.

The title compound, $[Cu(C_5H_3N_6)_2(H_2O)_2]\cdot 2C_5H_3N_3$, is a 1:2 co-crystal between the mononuclear complex diaquabis[5-(pyrazin-2-yl)tetrazolato]copper(II) and the reagent pyrazine-2-carbonitrile which was used in the synthesis. The Cu^{II} atom is located on an inversion centre and has a distorted octahedral [4 + 2]-coordination environment formed by four N atoms of two chelating bidentate 5-(pyrazin-2-yl)tetrazolate ligands at shorter distances and two water O atoms at longer distances. The Cu^{II} complex molecules are held together by O—H···N hydrogen bonds and π–π stacking interactions [centroid–centroid distance 3.6139 (8) Å], forming layers parallel to (100). These layers alternate with layers of pyrazine-2-carbonitrile molecules and both are held together *via* C—H···N hydrogen bonds and further π–π stacking interactions.

Related literature

For related Cu^{II} complexes, see: Liu *et al.* (2007); Abu-Youssef *et al.* (2007). For hydrogen-bonding networks and IR spectroscopy of related complexes, see: Abu-Youssef *et al.* (2007). For the synthesis of the title compound, see: Zhao *et al.* (2008).



Experimental

Crystal data

$[Cu(C_5H_3N_6)_2(H_2O)_2]\cdot 2C_5H_3N_3$
M_r = 604.06
Monoclinic, $P2_1/c$
a = 13.591 (2) Å
b = 12.784 (3) Å
c = 7.216 (2) Å
β = 104.93 (2)°
V = 1211.4 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.96 mm^{-1}
T = 100 K
0.10 × 0.08 × 0.06 mm

Data collection

Agilent SuperNova CCD diffractometer
72054 measured reflections
3711 independent reflections
3265 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.075
S = 1.08
3711 reflections
195 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu1—N3	1.9853 (9)	Cu1—O1	2.3477 (9)
Cu1—N2	2.0583 (10)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1W···N5^{i}	0.80 (2)	2.07 (2)	2.8577 (13)	170 (2)
O1—H2W···N6^{ii}	0.81 (1)	2.05 (1)	2.8543 (14)	173 (2)
C1—H1···N9^{iii}	0.95	2.57	3.2993 (17)	134
C3—H3···N4	0.95	2.51	3.2825 (15)	138
C11—H11···N1^{iv}	0.95	2.51	3.2800 (17)	138

Symmetry codes: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $-x+2, y-\frac{1}{2}, -z+\frac{5}{2}$; (iii) $x, -y-\frac{1}{2}, z-\frac{1}{2}$; (iv) $-x+1, -y, -z+1$.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2008); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2009).

Technical support (X-ray measurements) from CRM2 UMR-CNRS 7036 Jean Barriol Institut, Lorraine University, is gratefully acknowledged.

Supporting information for this paper is available from the IUCr electronic archives (Reference: QK2063).

References

Abu-Youssef, M. A. M., Mautner, F. A., Massoud, A. A. & Ohrstrom, L. (2007). *Polyhedron*, **26**, 1531–1540.
Burla, M. C., Camalli, M., Carrozzini, B., Cascarano, G. L., Giacovazzo, C., Polidori, G. & Spagna, R. (2003). *J. Appl. Cryst.* **36**, 1103.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Liu, J.-T., Fan, S.-D. & Ng, S. W. (2007). *Acta Cryst.* E**63**, m1651.

Oxford Diffraction, (2008). *CrysAlis PRO*. Oxford Diffraction Ltd, Yarnton, England.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Zhao, H., Qu, Z.-R., Ye, H.-Y. & Xiong, R.-G. (2008). *Chem. Soc. Rev.* **37**, 84–100.

supporting information

Acta Cryst. (2014). E**70**, m80–m81 [doi:10.1107/S1600536814002293]

Diaquabis[5-(2-pyrazin-2-yl)tetrazolato]copper(II)–pyrazine-2-carbonitrile (1/2)

Mohamed Abdellatif Bensegueni, Aouatef Cherouana, Slimane Dahaoui and Issam Boudraa

S1. Comment

In continuation of related research (Abu-Youssef *et al.*, 2007; Liu *et al.*, 2007), we set out to investigate a new copper compound with the aim to study its molecular and crystal structure including hydrogen bonding and network topology. The title compound, $[Cu(Pyztz)_2(H_2O)_2].(CPy)_2$ (Fig. 1), crystallizes in the monoclinic space group $P2_1/c$, and the asymmetric unit contains an anionic 5-(pyrazin-2-yl)tetrazolato ligand (Pyztz), one coordinated water molecule, one central Cu^{2+} ion which is located on an inversion centre, and one pyrazine-2-carbonitrile molecule (CPy). In the complex $[Cu(Pyztz)_2(H_2O)_2]$ the copper ion adopts a Jahn-Teller-distorted octahedral coordination by four N atoms of two chelating bidentate Pyztz ligands and by two water O atoms at distinctly longer distances (Table 1). The two Pyztz ligands of the complex are essentially coplanar and the complex is reinforced by two intramolecular hydrogen bonds C3—H3···N4 (Table 2). Identical Cu complexes with bond lengths similar to the title compound were reported from $[Cu(Pyztz)_2(H_2O)_2]$ (Abu-Youssef *et al.*, 2007) and from $[Cu(Pyztz)_2(H_2O)_2].H_2O$ (Liu *et al.*, 2007; Abu-Youssef *et al.*, 2007).

The $[Cu(Pyztz)_2(H_2O)_2]$ complexes in the title compound are arranged in layers parallel (100) and form two-dimensional infinite networks parallel this plane (Fig. 2). They are held together by O—H···N hydrogen bonds between the water molecules as donors and tetrazole nitrogen atoms N5 and N6 as acceptors (Table 2) and by π-π stacking interactions between pairs of tetrazole rings (Fig. 3; Cg3···Cg3). Inserted between the layers of the $[Cu(Pyztz)_2(H_2O)_2]$ complexes are layers of CPy molecules, which are held together by π-π stacking (Fig. 3, Cg5···Cg5) and by weak intermolecular C—H···N hydrogen bonds to N4 and N9 as acceptors (Fig. 2, Table 2).

From the topological viewpoint the structure of $[Cu(Pyztz)_2(H_2O)_2].(CPy)_2$ may be considered as tetragonal plane net, the Cu complex could be regarded as node. Each complex is bound to four other complexes and acting as 4-connected node and each cyanopyrazine fragment is between two tetragonal planes net. In this way the structure could be reduced to an uninodal 4 - c net, of sql topological type, and the Point (Schlafli) symbol for the net is $4^4\,6^2$ (Fig. 2 b).

S2. Experimental

The compound was prepared under solvothermal conditions, by a mixture of 0.065 g (1 mmol) of sodium azide, 2 ml of pyrazine-2-carbonitrile and 0.255 g (1 mmol) of copper fluoborate hydrate according to a literature procedure.(Zhao *et al.*, 2008). The mixture was kept indisturbed for a few days at room temperature and furnished blue crystals suitable for X-ray diffraction.

S3. Refinement

Carbon bonded H atoms were placed at calculated positions and were treated as riding on the parent C atoms with C—H = 0.95 Å, U_{iso}(H) = 1.2U_{eq}(C). The two H atoms of the water molecule were refined with distance restraints of O—H = 0.82 (1) Å and H–H = 1.40 (2) Å, whereas their U_{iso}(H) were refined freely.

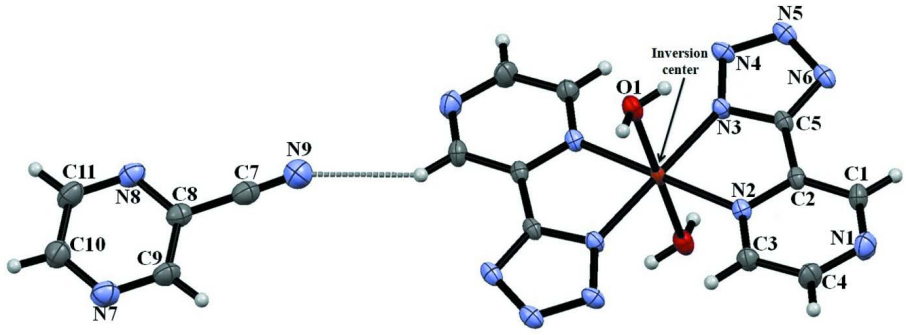


Figure 1

Molecular structure of the title compound $[Cu(Pyztz)_2(H_2O)_2].(CPy)_2$ with displacement ellipsoids drawn at the 50% probability level.

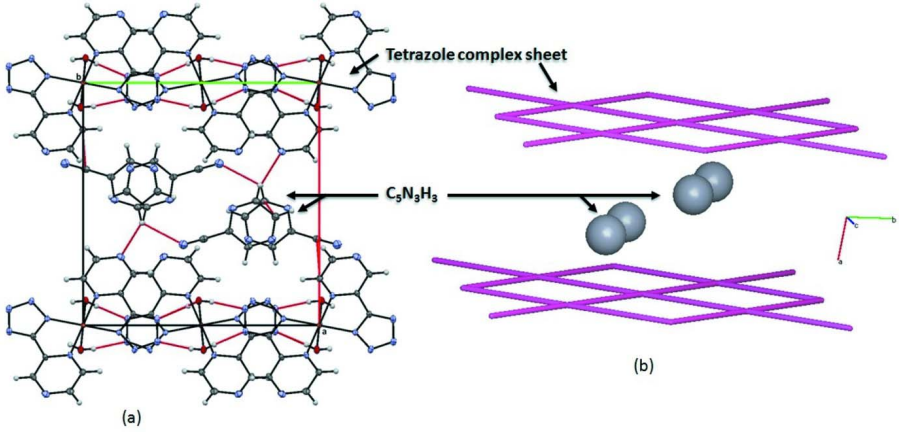


Figure 2

(*a*) The crystal structure of $[Cu(Pyztz)_2(H_2O)_2].(CPy)_2$ viewed along [001] showing hydrogen bonds as red lines. (*b*) The 4-connected sql net topology of the O—H···N hydrogen bonds in $[Cu(Pyztz)_2(H_2O)_2].(CPy)_2$.

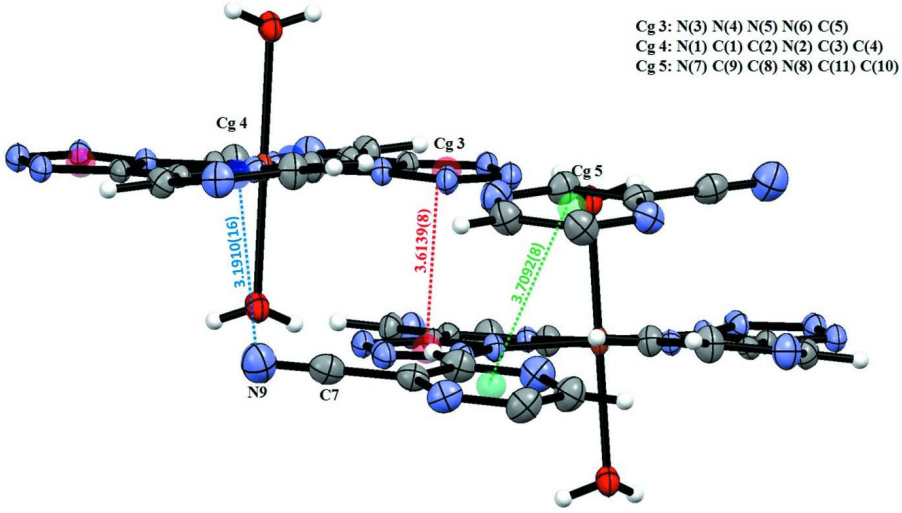


Figure 3

π-π stacking interactions in $[Cu(Pyztz)_2(H_2O)_2].(CPy)_2$ with Cg···Cg distances in Å.

Diaquabis[5-(2-pyrazin-2-yl)tetrazolato]copper(II)–pyrazine-2-carbonitrile (1/2)

Crystal data

$[Cu(C_5H_3N_6)_2(H_2O)_2]\cdot 2C_5H_3N_3$
$M_r = 604.06$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 13.591$ (2) Å
$b = 12.784$ (3) Å
$c = 7.216$ (2) Å
$\beta = 104.93$ (2)°
$V = 1211.4$ (5) Å^3
$Z = 2$
$F(000) = 614$
$D_x = 1.656$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 70 reflections
$\theta = 2.2$–$30.6°$
$\mu = 0.96$ mm^{-1}
$T = 100$ K
Prism, blue
0.1 × 0.08 × 0.06 mm

Data collection

Agilent SuperNova CCD diffractometer
Radiation source: micro-source
Multi-layer monochromator
φ and ω scans
72054 measured reflections
3711 independent reflections
3265 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 30.6°$, $\theta_{min} = 2.2°$
$h = -19\rightarrow19$
$k = -16\rightarrow18$
$l = -10\rightarrow10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.075$
$S = 1.08$
3711 reflections
195 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
$w = 1/[\sigma^2(F_o^2) + (0.0387P)^2 + 0.609P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.62$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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	1.0000	0.0000	1.0000	0.01027 (6)

O1	0.89916 (7)	−0.01043 (7)	1.21907 (13)	0.01521 (17)
H1W	0.9008 (14)	0.0452 (12)	1.271 (3)	0.022 (4)*
H2W	0.9197 (14)	−0.0577 (11)	1.294 (2)	0.028 (5)*
N1	0.71720 (8)	−0.15880 (9)	0.54002 (16)	0.0195 (2)
N2	0.87742 (8)	−0.05530 (7)	0.79219 (14)	0.01180 (18)
N3	0.97170 (8)	0.15216 (7)	0.96694 (14)	0.01155 (18)
N4	0.90083 (8)	0.21867 (8)	0.86795 (14)	0.01393 (19)
N5	0.93288 (8)	0.31435 (8)	0.91544 (15)	0.01499 (19)
N6	1.02487 (8)	0.31291 (8)	1.04561 (15)	0.01458 (19)
N7	0.64661 (9)	0.29939 (9)	0.97445 (17)	0.0217 (2)
N8	0.51739 (8)	0.13314 (9)	0.80887 (16)	0.0188 (2)
N9	0.66710 (10)	−0.07623 (10)	0.97158 (19)	0.0269 (3)
C1	0.78740 (9)	−0.21147 (9)	0.67013 (17)	0.0155 (2)
H1	0.7816	−0.2853	0.6786	0.019*
C2	0.86881 (9)	−0.16041 (8)	0.79360 (16)	0.0115 (2)
C3	0.80715 (10)	−0.00197 (9)	0.66417 (17)	0.0148 (2)
H3	0.8108	0.0722	0.6597	0.018*
C4	0.72809 (10)	−0.05505 (10)	0.53648 (18)	0.0186 (2)
H4	0.6802	−0.0157	0.4434	0.022*
C5	1.04598 (9)	0.21169 (8)	1.07398 (16)	0.0116 (2)
C7	0.64409 (10)	0.01012 (10)	0.9505 (2)	0.0195 (2)
C8	0.61209 (9)	0.11813 (10)	0.91986 (17)	0.0165 (2)
C9	0.67664 (10)	0.19991 (10)	1.00151 (18)	0.0191 (2)
H9	0.7432	0.1845	1.0778	0.023*
C10	0.55197 (10)	0.31480 (11)	0.86613 (19)	0.0214 (3)
H10	0.5274	0.3845	0.8444	0.026*
C11	0.48782 (10)	0.23276 (11)	0.78358 (19)	0.0210 (2)
H11	0.4213	0.2483	0.7073	0.025*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.01191 (10)	0.00595 (9)	0.01099 (10)	−0.00037 (6)	−0.00058 (7)	−0.00041 (6)
O1	0.0205 (4)	0.0105 (4)	0.0139 (4)	−0.0007 (3)	0.0032 (3)	−0.0003 (3)
N1	0.0178 (5)	0.0192 (5)	0.0187 (5)	−0.0033 (4)	0.0000 (4)	−0.0030 (4)
N2	0.0139 (4)	0.0097 (4)	0.0116 (4)	−0.0010 (3)	0.0028 (3)	−0.0009 (3)
N3	0.0138 (4)	0.0090 (4)	0.0110 (4)	0.0004 (3)	0.0016 (3)	0.0002 (3)
N4	0.0170 (5)	0.0104 (4)	0.0142 (4)	0.0030 (3)	0.0035 (4)	0.0020 (3)
N5	0.0197 (5)	0.0104 (4)	0.0155 (5)	0.0016 (4)	0.0057 (4)	0.0009 (3)
N6	0.0202 (5)	0.0089 (4)	0.0158 (4)	−0.0004 (4)	0.0068 (4)	−0.0004 (3)
N7	0.0188 (5)	0.0222 (5)	0.0225 (5)	−0.0026 (4)	0.0024 (4)	−0.0030 (4)
N8	0.0151 (5)	0.0225 (5)	0.0176 (5)	−0.0017 (4)	0.0020 (4)	−0.0032 (4)
N9	0.0231 (6)	0.0247 (6)	0.0316 (6)	−0.0003 (5)	0.0044 (5)	0.0031 (5)
C1	0.0168 (5)	0.0135 (5)	0.0154 (5)	−0.0044 (4)	0.0026 (4)	−0.0028 (4)
C2	0.0141 (5)	0.0103 (5)	0.0107 (5)	−0.0020 (4)	0.0042 (4)	−0.0015 (4)
C3	0.0159 (5)	0.0133 (5)	0.0139 (5)	0.0002 (4)	0.0014 (4)	0.0005 (4)
C4	0.0171 (6)	0.0186 (6)	0.0164 (6)	−0.0002 (4)	−0.0023 (4)	−0.0004 (4)
C5	0.0155 (5)	0.0087 (5)	0.0117 (5)	−0.0013 (4)	0.0051 (4)	−0.0004 (4)

C7	0.0153 (6)	0.0248 (6)	0.0178 (6)	−0.0019 (4)	0.0032 (4)	0.0007 (5)
C8	0.0154 (5)	0.0199 (6)	0.0141 (5)	−0.0015 (4)	0.0038 (4)	−0.0002 (4)
C9	0.0144 (5)	0.0228 (6)	0.0184 (6)	−0.0025 (4)	0.0012 (4)	−0.0009 (5)
C10	0.0196 (6)	0.0209 (6)	0.0225 (6)	0.0011 (5)	0.0033 (5)	−0.0019 (5)
C11	0.0153 (6)	0.0246 (6)	0.0207 (6)	0.0010 (5)	0.0005 (5)	−0.0030 (5)

Geometric parameters (Å, º)

Cu1—N3	1.9853 (9)	N7—C10	1.3365 (17)
Cu1—N3^{i}	1.9853 (9)	N8—C11	1.3338 (17)
Cu1—N2	2.0583 (10)	N8—C8	1.3431 (16)
Cu1—N2^{i}	2.0583 (10)	N9—C7	1.1467 (17)
Cu1—O1	2.3477 (9)	C1—C2	1.3915 (15)
Cu1—O1^{i}	2.3477 (9)	C1—H1	0.9500
O1—H1W	0.801 (17)	C2—C5^{i}	1.4538 (16)
O1—H2W	0.810 (13)	C3—C4	1.3978 (17)
N1—C4	1.3355 (16)	C3—H3	0.9500
N1—C1	1.3355 (16)	C4—H4	0.9500
N2—C3	1.3325 (15)	C5—C2^{i}	1.4538 (16)
N2—C2	1.3491 (14)	C7—C8	1.4475 (18)
N3—C5	1.3390 (15)	C8—C9	1.3940 (17)
N3—N4	1.3441 (13)	C9—H9	0.9500
N4—N5	1.3139 (14)	C10—C11	1.3955 (19)
N5—N6	1.3567 (15)	C10—H10	0.9500
N6—C5	1.3299 (14)	C11—H11	0.9500
N7—C9	1.3346 (18)		

N3—Cu1—N3^{i}	180.0	C11—N8—C8	115.26 (11)
N3—Cu1—N2^{i}	81.16 (4)	N1—C1—C2	121.32 (11)
N3^{i}—Cu1—N2^{i}	98.84 (4)	N1—C1—H1	119.3
N3—Cu1—N2	98.84 (4)	C2—C1—H1	119.3
N3^{i}—Cu1—N2	81.16 (4)	N2—C2—C1	121.24 (11)
N2^{i}—Cu1—N2	180.0	N2—C2—C5^{i}	113.46 (10)
N3—Cu1—O1	90.45 (4)	C1—C2—C5^{i}	125.21 (10)
N3^{i}—Cu1—O1	89.55 (4)	N2—C3—C4	120.04 (11)
N2^{i}—Cu1—O1	91.85 (4)	N2—C3—H3	120.0
N2—Cu1—O1	88.15 (4)	C4—C3—H3	120.0
N3—Cu1—O1^{i}	89.55 (4)	N1—C4—C3	122.66 (11)
N3^{i}—Cu1—O1^{i}	90.45 (4)	N1—C4—H4	118.7
N2^{i}—Cu1—O1^{i}	88.15 (4)	C3—C4—H4	118.7
N2—Cu1—O1^{i}	91.85 (4)	N6—C5—N3	111.32 (10)
O1—Cu1—O1^{i}	180.0	N6—C5—C2^{i}	130.06 (10)
Cu1—O1—H1W	108.3 (13)	N3—C5—C2^{i}	118.51 (10)
Cu1—O1—H2W	109.2 (13)	N9—C7—C8	178.22 (15)
H1W—O1—H2W	112.8 (17)	N8—C8—C9	123.16 (12)
C4—N1—C1	116.84 (11)	N8—C8—C7	115.56 (11)
C3—N2—C2	117.82 (10)	C9—C8—C7	121.28 (11)
C3—N2—Cu1	129.08 (8)	N7—C9—C8	121.16 (12)

C2—N2—Cu1	113.08 (8)	N7—C9—H9	119.4
C5—N3—N4	106.12 (9)	C8—C9—H9	119.4
C5—N3—Cu1	113.18 (8)	N7—C10—C11	122.70 (13)
N4—N3—Cu1	140.70 (8)	N7—C10—H10	118.6
N5—N4—N3	107.83 (10)	C11—C10—H10	118.6
N4—N5—N6	110.64 (9)	N8—C11—C10	121.74 (12)
C5—N6—N5	104.10 (9)	N8—C11—H11	119.1
C9—N7—C10	115.97 (12)	C10—C11—H11	119.1
N3—Cu1—N2—C3	5.57 (11)	C3—N2—C2—C5^{i}	174.67 (10)
N3^{i}—Cu1—N2—C3	−174.43 (11)	Cu1—N2—C2—C5^{i}	−6.64 (12)
O1—Cu1—N2—C3	95.74 (11)	N1—C1—C2—N2	2.97 (18)
O1^{i}—Cu1—N2—C3	−84.25 (11)	N1—C1—C2—C5^{i}	−173.49 (11)
N3—Cu1—N2—C2	−172.94 (8)	C2—N2—C3—C4	−0.28 (17)
N3^{i}—Cu1—N2—C2	7.06 (8)	Cu1—N2—C3—C4	−178.73 (9)
O1—Cu1—N2—C2	−82.77 (8)	C1—N1—C4—C3	−1.44 (19)
O1^{i}—Cu1—N2—C2	97.24 (8)	N2—C3—C4—N1	2.2 (2)
N2^{i}—Cu1—N3—C5	6.01 (8)	N5—N6—C5—N3	0.31 (13)
N2—Cu1—N3—C5	−173.99 (8)	N5—N6—C5—C2^{i}	−175.83 (11)
O1—Cu1—N3—C5	97.81 (8)	N4—N3—C5—N6	−0.29 (13)
O1^{i}—Cu1—N3—C5	−82.19 (8)	Cu1—N3—C5—N6	179.06 (7)
N2^{i}—Cu1—N3—N4	−174.98 (13)	N4—N3—C5—C2^{i}	176.35 (10)
N2—Cu1—N3—N4	5.01 (13)	Cu1—N3—C5—C2^{i}	−4.31 (13)
O1—Cu1—N3—N4	−83.19 (12)	C11—N8—C8—C9	−1.01 (18)
O1^{i}—Cu1—N3—N4	96.82 (12)	C11—N8—C8—C7	179.02 (12)
C5—N3—N4—N5	0.14 (12)	C10—N7—C9—C8	0.21 (19)
Cu1—N3—N4—N5	−178.91 (9)	N8—C8—C9—N7	0.7 (2)
N3—N4—N5—N6	0.05 (13)	C7—C8—C9—N7	−179.38 (12)
N4—N5—N6—C5	−0.22 (13)	C9—N7—C10—C11	−0.7 (2)
C4—N1—C1—C2	−1.06 (18)	C8—N8—C11—C10	0.56 (19)
C3—N2—C2—C1	−2.18 (17)	N7—C10—C11—N8	0.3 (2)
Cu1—N2—C2—C1	176.51 (9)		

Symmetry code: (i) −*x*+2, −*y*, −*z*+2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*W*···N5^{ii}	0.80 (2)	2.07 (2)	2.8577 (13)	170 (2)
O1—H2*W*···N6^{iii}	0.81 (1)	2.05 (1)	2.8543 (14)	173 (2)
C1—H1···N9^{iv}	0.95	2.57	3.2993 (17)	134
C3—H3···N4	0.95	2.51	3.2825 (15)	138
C11—H11···N1^{v}	0.95	2.51	3.2800 (17)	138

Symmetry codes: (ii) *x*, −*y*+1/2, *z*+1/2; (iii) −*x*+2, *y*−1/2, −*z*+5/2; (iv) *x*, −*y*−1/2, *z*−1/2; (v) −*x*+1, −*y*, −*z*+1.