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Crystal structure of *trans*-diaquabis(1*H*-pyrazole-3-carboxylato-κ^2N,O)copper(II) dihydrate

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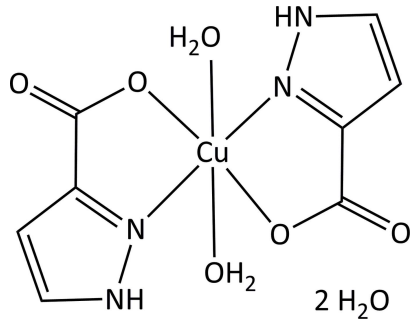
In the title compound, $[Cu(C_4H_3N_2O_2)_2(H_2O)_2]\cdot 2H_2O$, the Cu^{II} ion is located on an inversion centre and exhibits an axially elongated octahedral coordination geometry. The equatorial plane is formed by two *N*,*O*-bidentate 1*H*-pyrazole-3-carboxylate ligands in a *trans* configuration. The axial positions are occupied by two water molecules. The mononuclear complex molecules are arranged in layers parallel to the *ab* plane. Each complex molecule is linked to four adjacent species through intermolecular O—H···O and N—H···O hydrogen bonds that are established between the coordinating water molecules and carboxylate O atoms or protonated N atoms of the organic ligands. These layers are further connected into a three-dimensional network by additional hydrogen bonds involving solvent water molecules and non-coordinating carboxylate O atoms.

Keywords: crystal structure; copper(II) complex; *trans* configuration; 1*H*-pyrazole-3-carboxylate.

CCDC reference: 1437048

1. Related literature

For mononuclear cobalt(II), nickel(II) and zinc complexes of the 1*H*-pyrazole-3-carboxylate ligand, see: Artetxe *et al.* (2015); López-Viseras *et al.* (2014).



2. Experimental

2.1. Crystal data

$[Cu(C_4H_3N_2O_2)_2(H_2O)_2]\cdot 2H_2O$
M_r = 357.77
Monoclinic, $P2_1/c$
a = 6.4780 (4) Å
b = 21.5757 (10) Å
c = 4.8937 (3) Å
β = 105.856 (7)°
V = 657.96 (6) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 2.83 mm^{-1}
T = 100 K
0.09 × 0.04 × 0.02 mm

2.2. Data collection

Agilent SuperNova Single source at offset diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.817, T_{max} = 1
4452 measured reflections
1216 independent reflections
1089 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.074
S = 1.09
1216 reflections
109 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N2	1.9808 (16)	Cu1—O1*W*	2.4501 (15)
Cu1—O7	1.9910 (14)		
N2—Cu1—O7	81.30 (6)	O7—Cu1—O1*W*	89.43 (5)
N2—Cu1—O1*W*	92.08 (6)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1*W*^{i}	0.88	1.93	2.710 (2)	147
O1*W*—H1*WA*···O8^{ii}	0.83 (2)	1.86 (2)	2.667 (2)	163 (3)
O1*W*—H1*WB*···O7^{iii}	0.82 (2)	1.96 (2)	2.709 (2)	153 (3)
O2*W*—H2*WA*···O2*W*^{iv}	0.83 (2)	1.95 (2)	2.7792 (15)	178 (3)
O2*W*—H2*WB*···O8	0.81 (2)	2.04 (2)	2.854 (2)	175 (3)

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

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *OLEX2* (Dolomanov *et al.*, 2009); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: IM2473).

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supporting information

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Crystal structure of *trans*-diaquabis(1*H*-pyrazole-3-carboxylato-κ^2N,O)copper(II) dihydrate

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S1. Structural commentary

The title compound, $[Cu(C_4H_3N_2O_2)_2(H_2O)_2]\cdot 2H_2O$ crystallizes in the monoclinic crystal system, space group $P2_1/c$. The equatorial Cu—O and Cu—N distances (Table 1) are similar to those observed for the corresponding Co(II), Ni(II) and Zn(II) analogues (Artetxe *et al.*, 2015; López-Viseras *et al.*, 2014). However, the axial bond lenghts are much longer due to the Jahn-Teller effect operating in Cu(II) centres. The mononuclear complexes arrange in layers parallel to the *ab* plane through intermolecular O—H···O and N—H···O hydrogen bonds that are established between the coordinated water molecules (O1W) and carboxylate O atoms (O7, O8) or protonated N atoms (N2) of the organic ligands. These layers are further connected into a three-dimensional network by additional hydrogen bonds involving solvent water molecules (O2W) and non-coordinating carboxylate O atoms (O8). Table 2 summarizes the geometrical parameters of these O—H···O and N—H···O hydrogen bonding interactions.

S2. Synthesis and crystallization

To a solution of $CuCl_2\cdot 2\,H_2O$ (51 mg, 0.3 mmol) in hot water (15 ml) 1*H*-pyrazole-3-carboxylic acid (74 mg, 0.6 mmol) dissolved in hot water (10 ml) was added dropwise. After stirring for 30 min at 90 °C, the final solution was left undisturbed and prismatic blue crystals suitable for X-ray diffraction were obtained upon cooling to room temperature (Yield: 68 mg, 63%).

S3. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. All atoms except H were refined anisotropically. H atoms of the water molecules were located in a Fourier difference map and refined isotropically with O—H bond lenghts restrained to 0.84 (2) and with $U_{iso}(H) = 1.5U_{eq}(O)$. All pyrazole H atoms were positioned geometrically and refined using a riding model with C—H = 0.95 Å, N—H = 0.88 Å and $U_{iso}(H) = 1.2U_{eq}(C,N)$.

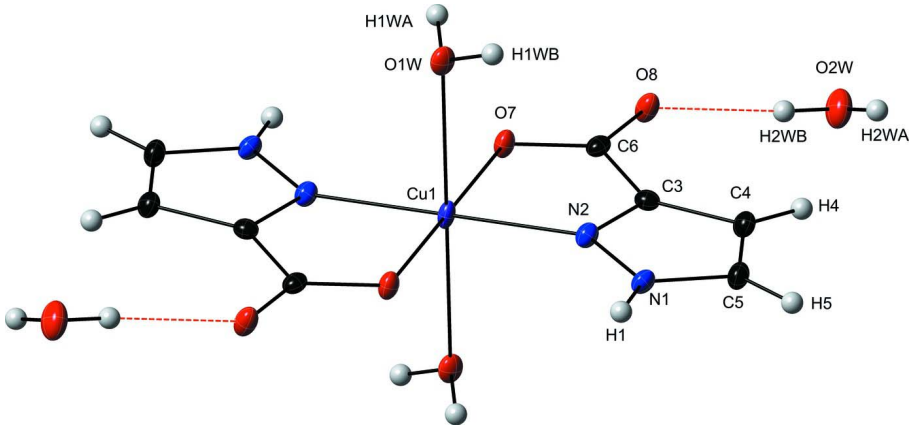

Figure 1

Molecular structure of $[Cu(C_4H_3N_2O_2)_2(H_2O)_2]\cdot 2H_2O$ showing the atom labelling for the asymmetric unit and 50% probability displacement ellipsoids.

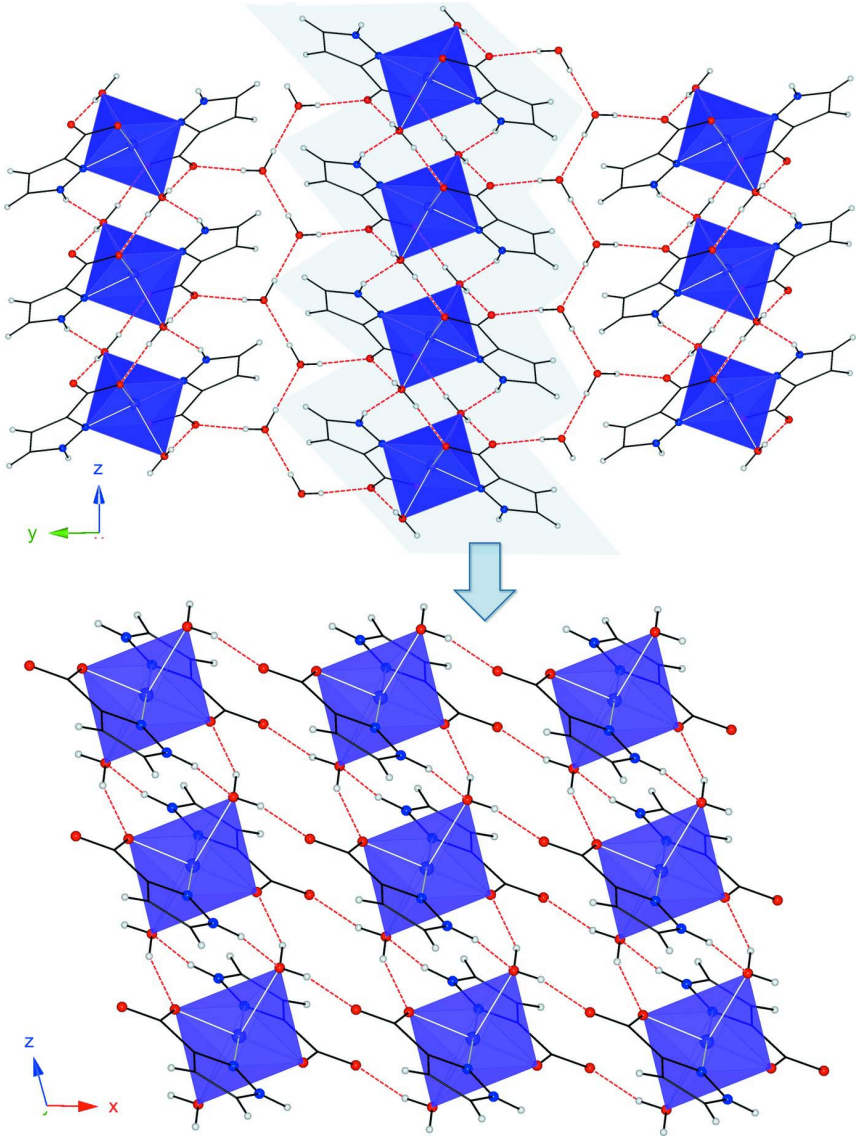

Figure 2

View of the crystal packing along the crystallographic *a* axis (above). Projection of a layer of $[Cu(C_4H_3N_2O_2)_2(H_2O)_2]$ complexes along the [010] direction (below). Cu(II) centres are represented as translucent octahedra and the O—H···O and N—H···O hydrogen bonds are depicted as dashed red lines.

trans-Diaquabis(1*H*-pyrazole-3-carboxylato-κ^2N,O)copper(II) dihydrate

Crystal data

$[Cu(C_4H_3N_2O_2)_2(H_2O)_2]\cdot 2H_2O$
$M_r = 357.77$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 6.4780\ (4)$ Å
$b = 21.5757\ (10)$ Å
$c = 4.8937\ (3)$ Å
$\beta = 105.856\ (7)°$
$V = 657.96\ (6)$ Å^3
$Z = 2$
$F(000) = 366$
$D_x = 1.806$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 1956 reflections
$\theta = 4.1–73.7°$
$\mu = 2.83$ mm^{-1}

T = 100 K
Prism, blue
0.09 × 0.04 × 0.02 mm

Data collection

Agilent SuperNova Single source at offset diffractometer
Radiation source: SuperNova (Cu) X-ray Source
Mirror monochromator
Detector resolution: 5.2012 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.817, T_{max} = 1
4452 measured reflections
1216 independent reflections
1089 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 69°, θ_{min} = 4.1°
h = −6→7
k = −23→26
l = −5→5

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.074
S = 1.09
1216 reflections
109 parameters
4 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
$w = 1/[\sigma^2(F_o^2) + (0.0406P)^2 + 0.2735P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Special details

Experimental. IR (KBr pellets, cm^{-1}): 3487(*s*), 3340(*s*), 3140(*s*), 3075(*s*), 2854(*s*), 2795(*s*), 1695(*s*), 1501(*m*), 1451(w), 1358(*s*), 1263(w), 1132(w), 1069(w), 1015(w), 943(*m*), 899(*m*), 839(*m*), 785(*m*), 648(*m*), 615(w), 500(w).
TGA/DTA (synthetic air, 5°C min^{-1}): The initial endothermic dehydration proccess (calcd/found for 4H_2O: 20.1 /20.2%) is completed at c.a. 85°C and is followed by a thermal stability range for the anydrous phase that extends up to c.a. 210°C. The highly exothermic ligand combustion results in the final residue at 370°C (calcd/found for CuO: 22.1/21.8%).
CHN (%m, calcd/found): C (26.8/27.2), H (3.9/3.9), N(15.7/15.5).

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	0.5	0.5	0	0.01043 (15)
N1	0.5203 (3)	0.37840 (7)	−0.3376 (4)	0.0113 (4)
H1	0.6239	0.3877	−0.4153	0.014*
N2	0.4416 (3)	0.41696 (7)	−0.1769 (4)	0.0111 (4)
C3	0.2890 (3)	0.38581 (9)	−0.0975 (4)	0.0105 (4)
C4	0.2691 (3)	0.32597 (9)	−0.2127 (4)	0.0124 (4)
H4	0.1732	0.2942	−0.1909	0.015*

C5	0.4182 (3)	0.32329 (9)	−0.3637 (4)	0.0137 (4)
H5	0.4452	0.2886	−0.4687	0.016*
C6	0.1815 (3)	0.42089 (9)	0.0858 (4)	0.0107 (4)
O7	0.2562 (2)	0.47569 (6)	0.1520 (3)	0.0118 (3)
O8	0.0330 (2)	0.39735 (6)	0.1641 (3)	0.0144 (3)
O1W	0.2455 (2)	0.54965 (6)	−0.4047 (3)	0.0134 (3)
O2W	−0.1631 (3)	0.28054 (7)	0.2052 (4)	0.0219 (4)
H1WA	0.140 (4)	0.5615 (13)	−0.353 (6)	0.033*
H1WB	0.208 (5)	0.5252 (12)	−0.536 (5)	0.033*
H2WA	−0.167 (5)	0.2621 (13)	0.054 (5)	0.033*
H2WB	−0.102 (4)	0.3132 (10)	0.201 (6)	0.033*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0144 (2)	0.0066 (2)	0.0126 (2)	−0.00226 (14)	0.00748 (17)	−0.00236 (15)
N1	0.0134 (8)	0.0095 (8)	0.0118 (8)	0.0020 (6)	0.0049 (7)	−0.0013 (6)
N2	0.0139 (8)	0.0095 (8)	0.0105 (8)	0.0006 (6)	0.0046 (7)	−0.0006 (6)
C3	0.0101 (9)	0.0116 (9)	0.0091 (9)	−0.0005 (7)	0.0016 (7)	0.0019 (7)
C4	0.0147 (10)	0.0089 (9)	0.0136 (10)	−0.0006 (8)	0.0039 (8)	0.0008 (7)
C5	0.0162 (10)	0.0094 (9)	0.0149 (10)	0.0008 (7)	0.0035 (8)	−0.0019 (7)
C6	0.0124 (9)	0.0098 (9)	0.0093 (10)	0.0026 (7)	0.0021 (8)	0.0013 (7)
O7	0.0153 (7)	0.0087 (6)	0.0132 (7)	−0.0015 (5)	0.0071 (5)	−0.0020 (5)
O8	0.0159 (7)	0.0106 (7)	0.0198 (8)	−0.0013 (5)	0.0103 (6)	0.0000 (6)
O1W	0.0153 (7)	0.0130 (7)	0.0140 (7)	−0.0010 (6)	0.0076 (6)	−0.0037 (6)
O2W	0.0313 (9)	0.0143 (7)	0.0209 (9)	−0.0057 (7)	0.0084 (7)	0.0011 (7)

Geometric parameters (Å, º)

Cu1—N2	1.9808 (16)	C3—C6	1.484 (3)
Cu1—N2^{i}	1.9808 (16)	C4—C5	1.369 (3)
Cu1—O7^{i}	1.9910 (14)	C4—H4	0.95
Cu1—O7	1.9910 (14)	C5—H5	0.95
Cu1—O1W	2.4501 (15)	C6—O8	1.238 (3)
Cu1—O1W^{i}	2.4501 (15)	C6—O7	1.285 (2)
N1—N2	1.338 (2)	O1W—H1WA	0.833 (18)
N1—C5	1.350 (3)	O1W—H1WB	0.817 (18)
N1—H1	0.88	O2W—H2WA	0.834 (18)
N2—C3	1.338 (3)	O2W—H2WB	0.813 (17)
C3—C4	1.401 (3)		
N2—Cu1—N2^{i}	180.00 (4)	N1—N2—Cu1	139.59 (13)
N2—Cu1—O7^{i}	98.70 (6)	N2—C3—C4	109.90 (18)
N2^{i}—Cu1—O7^{i}	81.30 (6)	N2—C3—C6	115.16 (17)
N2—Cu1—O7	81.30 (6)	C4—C3—C6	134.95 (18)
N2^{i}—Cu1—O7	98.70 (6)	C4—C3—Cu1	150.27 (15)
O7^{i}—Cu1—O7	180	C6—C3—Cu1	74.67 (11)
N2—Cu1—O1W	92.08 (6)	C5—C4—C3	104.79 (17)

N2^{i}—Cu1—O1W	87.92 (6)	C5—C4—H4	127.6
O7^{i}—Cu1—O1W	90.57 (5)	C3—C4—H4	127.6
O7—Cu1—O1W	89.43 (5)	N1—C5—C4	108.16 (18)
N2—Cu1—O1W^{i}	87.92 (6)	N1—C5—H5	125.9
N2^{i}—Cu1—O1W^{i}	92.08 (6)	C4—C5—H5	125.9
O7^{i}—Cu1—O1W^{i}	89.43 (5)	O8—C6—O7	124.79 (19)
O7—Cu1—O1W^{i}	90.57 (5)	O8—C6—C3	120.69 (17)
O1W—Cu1—O1W^{i}	180.00 (6)	O7—C6—C3	114.52 (17)
N2—N1—C5	110.36 (17)	O8—C6—Cu1	164.75 (15)
C5—N1—Cu1	134.42 (13)	C3—C6—Cu1	74.54 (11)
N2—N1—H1	124.8	C6—O7—Cu1	115.51 (13)
C5—N1—H1	124.8	Cu1—O1W—H1WA	108 (2)
Cu1—N1—H1	100.7	Cu1—O1W—H1WB	110 (2)
C3—N2—N1	106.79 (16)	H1WA—O1W—H1WB	110 (3)
C3—N2—Cu1	113.30 (14)	H2WA—O2W—H2WB	107 (3)

N2^{i}—Cu1—N1—N2	180	O7—Cu1—C3—C6	−0.48 (10)
O7^{i}—Cu1—N1—N2	−176.5 (2)	O1W—Cu1—C3—C6	−87.49 (11)
O7—Cu1—N1—N2	3.5 (2)	O1W^{i}—Cu1—C3—C6	92.51 (11)
O1W—Cu1—N1—N2	−86.4 (2)	N2—C3—C4—C5	0.2 (2)
O1W^{i}—Cu1—N1—N2	93.6 (2)	C6—C3—C4—C5	−180.0 (2)
N2—Cu1—N1—C5	−8.9 (2)	Cu1—C3—C4—C5	−6.1 (3)
N2^{i}—Cu1—N1—C5	171.1 (2)	N2—N1—C5—C4	−0.5 (2)
O7^{i}—Cu1—N1—C5	174.58 (18)	Cu1—N1—C5—C4	3.4 (3)
O7—Cu1—N1—C5	−5.42 (18)	C3—C4—C5—N1	0.2 (2)
O1W—Cu1—N1—C5	−95.26 (18)	N2—C3—C6—O8	177.59 (17)
O1W^{i}—Cu1—N1—C5	84.74 (18)	C4—C3—C6—O8	−2.3 (3)
C5—N1—N2—C3	0.6 (2)	Cu1—C3—C6—O8	−179.15 (18)
Cu1—N1—N2—C3	−172.7 (3)	N2—C3—C6—O7	−2.6 (3)
C5—N1—N2—Cu1	173.24 (16)	C4—C3—C6—O7	177.6 (2)
O7^{i}—Cu1—N2—C3	175.82 (13)	Cu1—C3—C6—O7	0.68 (14)
O7—Cu1—N2—C3	−4.18 (13)	N2—C3—C6—Cu1	−3.26 (14)
O1W—Cu1—N2—C3	−93.28 (14)	C4—C3—C6—Cu1	176.9 (2)
O1W^{i}—Cu1—N2—C3	86.72 (14)	N2—Cu1—C6—O8	179.6 (6)
O7^{i}—Cu1—N2—N1	3.5 (2)	N2^{i}—Cu1—C6—O8	−0.4 (6)
O7—Cu1—N2—N1	−176.5 (2)	O7^{i}—Cu1—C6—O8	176.3 (5)
O1W—Cu1—N2—N1	94.4 (2)	O7—Cu1—C6—O8	−3.7 (5)
O1W^{i}—Cu1—N2—N1	−85.6 (2)	O1W—Cu1—C6—O8	−88.9 (5)
N1—N2—C3—C4	−0.4 (2)	O1W^{i}—Cu1—C6—O8	91.1 (5)
Cu1—N2—C3—C4	−175.27 (13)	N2—Cu1—C6—O7	−176.66 (15)
N1—N2—C3—C6	179.66 (15)	N2^{i}—Cu1—C6—O7	3.34 (15)
Cu1—N2—C3—C6	4.8 (2)	O7^{i}—Cu1—C6—O7	180
N1—N2—C3—Cu1	174.8 (2)	O1W—Cu1—C6—O7	−85.20 (13)
N2^{i}—Cu1—C3—N2	180	O1W^{i}—Cu1—C6—O7	94.80 (13)
O7^{i}—Cu1—C3—N2	−5.02 (16)	N2—Cu1—C6—C3	2.38 (10)
O7—Cu1—C3—N2	174.98 (16)	N2^{i}—Cu1—C6—C3	−177.62 (10)
O1W—Cu1—C3—N2	87.97 (14)	O7^{i}—Cu1—C6—C3	−0.96 (19)
O1W^{i}—Cu1—C3—N2	−92.03 (14)	O7—Cu1—C6—C3	179.04 (19)

N2—Cu1—C3—C4	9.0 (2)	O1W—Cu1—C6—C3	93.84 (10)
N2^{i}—Cu1—C3—C4	−171.0 (2)	O1W^{i}—Cu1—C6—C3	−86.16 (10)
O7^{i}—Cu1—C3—C4	4.0 (3)	O8—C6—O7—Cu1	178.80 (15)
O7—Cu1—C3—C4	−176.0 (3)	C3—C6—O7—Cu1	−1.0 (2)
O1W—Cu1—C3—C4	97.0 (3)	N2—Cu1—O7—C6	2.83 (13)
O1W^{i}—Cu1—C3—C4	−83.0 (3)	N2^{i}—Cu1—O7—C6	−177.17 (13)
N2—Cu1—C3—C6	−175.5 (2)	O1W—Cu1—O7—C6	95.02 (13)
N2^{i}—Cu1—C3—C6	4.5 (2)	O1W^{i}—Cu1—O7—C6	−84.98 (13)
O7^{i}—Cu1—C3—C6	179.52 (10)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1*W*^{ii}	0.88	1.93	2.710 (2)	147
O1*W*—H1*WA*···O8^{iii}	0.83 (2)	1.86 (2)	2.667 (2)	163 (3)
O1*W*—H1*WB*···O7^{iv}	0.82 (2)	1.96 (2)	2.709 (2)	153 (3)
O2*W*—H2*WA*···O2*W*^{v}	0.83 (2)	1.95 (2)	2.7792 (15)	178 (3)
O2*W*—H2*WB*···O8	0.81 (2)	2.04 (2)	2.854 (2)	175 (3)

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