



Crystal structure of {2-methyl-2-[(pyridin-2-yl-methyl)amino]propan-1-ol- κ^3 N,N',O}bis(nitrato- κ O)copper(II) from synchrotron data

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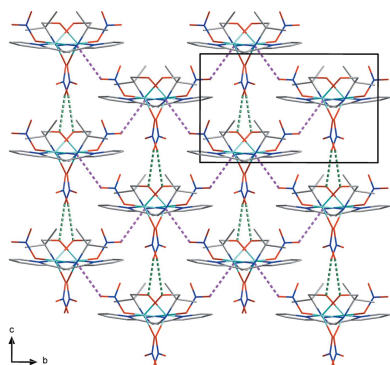
Keywords: crystal structure; π - π interaction; hydrogen bond; synchrotron data.**CCDC reference:** 1887447**Supporting information:** this article has supporting information at journals.iucr.org/e

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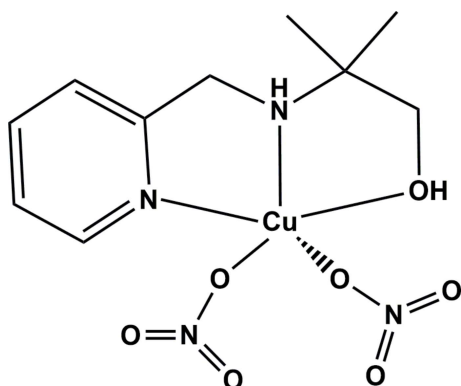
The title compound, [Cu(NO₃)₂(C₁₀H₁₆N₂O)], has been synthesized and characterized by synchrotron single-crystal diffraction at 100 K. The Cu^{II} ion has a distorted square-pyramidal coordination geometry with two N and one O atoms of the C₁₀H₁₆N₂O ligand and one nitrate anion in the equatorial plane and another nitrate anion at the axial position. The equatorial Cu–N and Cu–O bond lengths are in the range 1.9608 (14)–2.0861 (15) Å, which are shorter than the axial Cu–O_{nitrate} bond length [2.1259 (16) Å]. In the crystal, molecules are linked *via* intermolecular N–H...O and O–H...O hydrogen bonds, forming a sheet structure parallel to the *bc* plane. The sheets are further linked through a face-to-face π - π interaction [centroid-centroid distance = 3.994 (1) Å]. Weak intermolecular C–H...O interactions are also observed in the sheet and between adjacent sheets.

1. Chemical context

Transition-metal complexes containing amine or its derivative ligands have attracted considerable attention owing to their diverse coordination geometries and their various applications in catalysis (Ahn *et al.*, 2017), as magnetic materials (Liu, Zhou *et al.*, 2017) and fluorescent substances (Chia & Tay, 2014) as well as sensing materials (Liu, Wang *et al.*, 2017). In addition, polyamine ligands containing hydroxyl groups can easily form multinuclear complexes (such as dinuclear or trinuclear) with various transition-metal ions and hydrogen-bonded supramolecular compounds due to the deprotonation of hydroxyl groups by the transition-metal ions and anions (Shin *et al.*, 2014). For example, *N*-(2-pyridylmethyl)iminodiethanol and *N*-(2-pyridylmethyl)iminodiisopropanol ligands containing amine, pyridine and hydroxyl groups have been used to form trinuclear metal complexes with cobalt and nickel ions, respectively, and these complexes have shown significant olefin epoxidations and magnetic interactions (Shin, Jeong *et al.*, 2016). The nitrate anion is a good candidate for the construction of multinuclear complexes or supramolecular compounds by bridging metal ions or hydrogen bonding adjacent molecules (El-Khatib *et al.*, 2018). Here, we report the preparation and crystal structure of a copper(II) complex, [Cu(C₁₀H₁₆N₂O)(NO₃)₂], formed with a functional tridentate ligand, 2-methyl-2-[(2-pyridinylmethyl)amino]-1-propanol, and nitrate anions.



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2. Structural commentary

A view of the molecular structure of the title compound is shown in Fig. 1. The central Cu^{II} ion is coordinated by two nitrogen and one oxygen atoms from the C₁₀H₁₆N₂O ligand and by two oxygen atoms from nitrate anions, and adopts a distorted square-pyramidal geometry. The equatorial plane consists of the two nitrogen atoms (N1 and N2) and the oxygen atom (O1) of the hydroxyl group in the C₁₀H₁₆N₂O ligand and one oxygen atom (O5) of the nitrate anion. The coordination geometry is completed by an oxygen atom (O2) from the other nitrate anion in the axial position. The equatorial bond lengths, Cu–N and Cu–O, are in the range 1.9608 (14) to 2.0861 (15) Å. The axial bond length, Cu–O_{nitrate}, is 2.1259 (16) Å. The average length of the Cu–N and Cu–O bonds between the Cu^{II} ion and the C₁₀H₁₆N₂O ligand is 2.0081 (8) Å, which is shorter than the average bond length in the reported [Cu(C₁₀H₁₆N₂O)Cl₂] complex possessing the same ligand and metal (Shin, Lee *et al.*, 2016). The axial bond

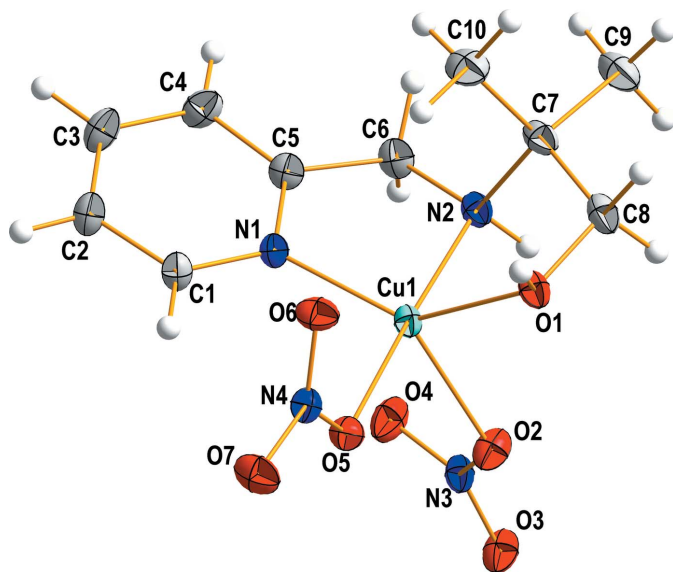


Figure 1
View of the molecular structure of the title compound, showing the atom-labelling scheme, with displacement ellipsoids drawn at the 50% probability.

Table 1
Hydrogen-bond geometry (Å, °).

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
O1–H1O1···O3 ⁱ	0.83 (1)	1.89 (2)	2.685 (2)	159 (4)
N2–H2···O7 ⁱⁱ	0.98 (1)	1.97 (2)	2.930 (3)	167 (3)
C4–H4···O2 ⁱⁱⁱ	0.95	2.31	3.204 (3)	156
C8–H8A···O5 ^{iv}	0.99	2.55	3.455 (3)	152

Symmetry codes: (i) $x, y, z + 1$; (ii) $-x + \frac{3}{2}, y + \frac{1}{2}, z - \frac{1}{2}$; (iii) $x - \frac{1}{2}, -y + \frac{3}{2}, z$; (iv) $-x + \frac{3}{2}, y + \frac{1}{2}, z + \frac{1}{2}$.

length is also shorter than that in [Cu(C₁₀H₁₆N₂O)Cl₂], which can be attributed to the size effect of the coordinated anions. The nitrate anions are coordinated in a *cis* position to each other and the axial bond is longer than the equatorial bond. The bite angles N1–Cu1–N2 and N2–Cu1–O1 in the five-membered chelate rings are 84.53 (7) and 82.92 (7)°, respectively.

3. Supramolecular features

In the crystal, two nitrate anions form intermolecular hydrogen bonds (O1–H1O1···O3ⁱ, N2–H2···O7ⁱⁱ and C8–H8A···O5^{iv}; symmetry codes as in Table 1) with adjacent C₁₀H₁₆N₂O ligands, generating an undulating sheet structure parallel to the *bc* plane (Fig. 2). Another C–H···O hydrogen bond (C4–H4···O2ⁱⁱⁱ; Table 1) links the sheets into a three-dimensional structure (Fig. 3). Moreover, the sheets are linked by a π – π interaction between pyridine rings; the distance between the centroids of the pyridine rings is 3.994 (1) Å and the dihedral angle is 19.317 (1)°.

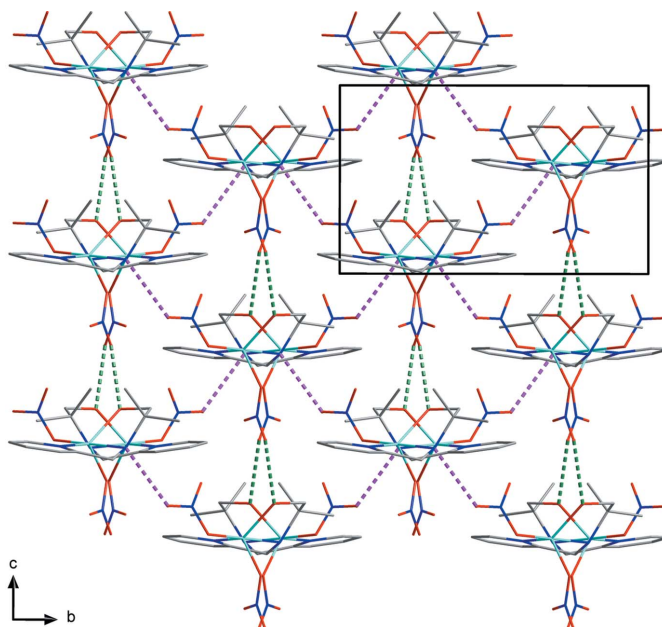


Figure 2
A packing diagram of the title compound viewed along the *a* axis, showing the N–H···O (purple dashed lines) and O–H···O (dark green dashed lines) hydrogen bonds.

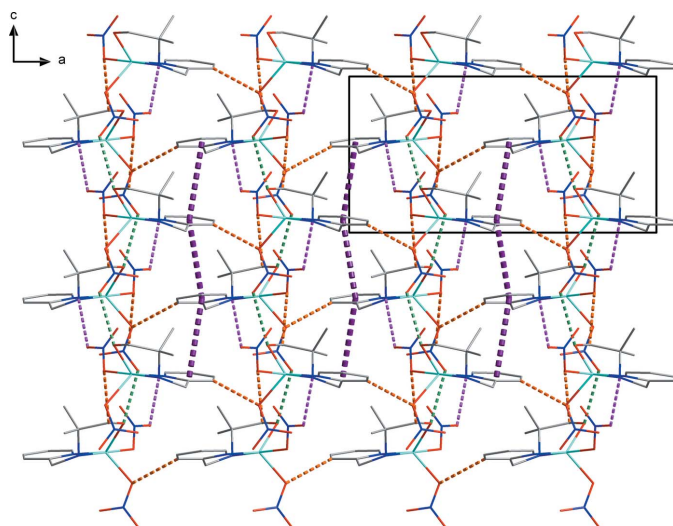


Figure 3
A packing diagram of the title compound viewed along the *b* axis, showing the N–H···O (purple dashed lines), O–H···O (dark green dashed lines) and C–H···O (orange dashed lines) hydrogen bonds as well as π – π interactions (violet dashed lines).

4. Database survey

A search of the Cambridge Structural Database (Version 5.39, update of August 2018; Groom *et al.*, 2016) shows only one mononuclear copper(II) complex with the same $C_{10}H_{16}N_2O$ ligand, for which the synthesis and crystal structure have been reported (Shin, Lee *et al.*, 2016). A similar copper(II) complex with poly(2,6-dimethyl-1,4-phenylene ether) ligands involving secondary amine, pyridine and hydroxyl groups has been prepared to study its catalytic activities (Guieu *et al.*, 2004).

5. Synthesis and crystallization

The $C_{10}H_{16}N_2O$ ligand was prepared according to a slight modification of the previous reported method (Shin, Lee *et al.*, 2016). To a methanol solution (10 mL) of $Cu(NO_3)_2 \cdot 3H_2O$ (200 mg, 0.823 mmol) was added dropwise a methanol solution (10 mL) of $C_{10}H_{16}N_2O$ (149 mg, 0.823 mmol); the colour became dark blue, and the solution was stirred for 30 min at room temperature. Blue crystals of the title compound were obtained by diffusion of diethyl ether into the dark-blue solution for several days, and collected by filtration and washed with diethyl ether and dried in air (yield: 189 mg, 62%). FT-IR(ATR, cm^{-1}): 3215, 3168, 3071, 2967, 1607, 1506, 1384, 1278, 1065, 1020.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. C-bound H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C–H = 0.95–0.99 Å, and with $U_{iso}(H) = 1.5$ or $1.2U_{eq}(C)$. The positions of the O- and N-bound H atoms were assigned based on a difference-Fourier map, and

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Cu(NO_3)_2(C_{10}H_{16}N_2O)]$
M_r	367.81
Crystal system, space group	Orthorhombic, $Pna2_1$
Temperature (K)	100
a, b, c (Å)	14.990 (3), 12.520 (3), 7.6290 (15)
V (Å ³)	1431.8 (5)
Z	4
Radiation type	Synchrotron, $\lambda = 0.630$ Å
μ (mm ⁻¹)	1.13
Crystal size (mm)	0.11 × 0.10 × 0.08
Data collection	
Diffractometer	ADSC Q210 CCD area detector
Absorption correction	Empirical (using intensity measurements) (<i>HKL3000sm SCALEPACK</i> ; Otwinowski & Minor, 1997)
T_{min}, T_{max}	0.912, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	13671, 4431, 4234
R_{int}	0.032
$(\sin \theta/\lambda)_{max}$ (Å ⁻¹)	0.720
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.025, 0.066, 1.08
No. of reflections	4431
No. of parameters	208
No. of restraints	3
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å ⁻³)	0.40, -0.68
Absolute structure	Flack x determined using 1883 quotients $[(I^+) - (I^-)] / [(I^+) + (I^-)]$ (Parsons <i>et al.</i> , 2013)
Absolute structure parameter	0.037 (5)

Computer programs: *PAL BL2D-SMDC* (Shin, Eom *et al.*, 2016), *HKL3000sm* (Otwinowski & Minor, 1997), *SHELXT2014* (Sheldrick, 2015a), *SHELXL2018* (Sheldrick, 2015b), *DIAMOND* (Putz & Brandenburg, 2014) and *publCIF* (Westrip, 2010).

were refined with distance restraints of O–H = 0.84 (1) Å and N–H = 1.00 (1) Å, and with $U_{iso}(H) = 1.5U_{eq}(O)$ and $1.2U_{eq}(N)$. One reflection with a poor agreement between the measured and calculated intensities was omitted from the final refinement cycles.

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Crystal structure of {2-methyl-2-[(pyridin-2-ylmethyl)amino]propan-1-ol- κ^3N,N',O }bis(nitrato- κO)copper(II) from synchrotron data

Jong Won Shin, Dae-Woong Kim, Jae-Woo Jeon and Dohyun Moon

Computing details

Data collection: *PAL BL2D-SMDC* (Shin, Eom *et al.*, 2016); cell refinement: *HKL3000sm* (Otwinowski & Minor, 1997); data reduction: *HKL3000sm* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXT2014* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015b); molecular graphics: *DIAMOND* (Putz & Brandenburg, 2014); software used to prepare material for publication: *publCIF* (Westrip, 2010).

{2-Methyl-2-[(pyridin-2-ylmethyl)amino]propan-1-ol- κ^3N,N',O }bis(nitrato- κO)copper(II)

Crystal data

[Cu(NO₃)₂(C₁₀H₁₆N₂O)]

$M_r = 367.81$

Orthorhombic, *Pna*2₁

$a = 14.990$ (3) Å

$b = 12.520$ (3) Å

$c = 7.6290$ (15) Å

$V = 1431.8$ (5) Å³

$Z = 4$

$F(000) = 756$

$D_x = 1.706$ Mg m⁻³

Synchrotron radiation, $\lambda = 0.630$ Å

Cell parameters from 29915 reflections

$\theta = 0.4$ – 33.6°

$\mu = 1.13$ mm⁻¹

$T = 100$ K

Block, blue

$0.11 \times 0.10 \times 0.08$ mm

Data collection

ADSC Q210 CCD area detector
diffractometer

Radiation source: PLSII 2D bending magnet

ω scan

Absorption correction: empirical (using
intensity measurements)

(*HKL3000sm SCALEPACK*; Otwinowski &
Minor, 1997)

$T_{\min} = 0.912$, $T_{\max} = 1.000$

13671 measured reflections

4431 independent reflections

4234 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.032$

$\theta_{\max} = 27.0^\circ$, $\theta_{\min} = 1.9^\circ$

$h = -21 \rightarrow 21$

$k = -18 \rightarrow 18$

$l = -10 \rightarrow 10$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.025$

$wR(F^2) = 0.066$

$S = 1.08$

4431 reflections

208 parameters

3 restraints

Hydrogen site location: mixed

H atoms treated by a mixture of independent
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0434P)^2 + 0.0982P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.002$

$\Delta\rho_{\max} = 0.40$ e Å⁻³

$\Delta\rho_{\min} = -0.68$ e Å⁻³

Extinction correction: *SHELXL2018* (Sheldrick,
2015b), $F_c^* = kF_c[1 + 0.001xF_c^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.026 (3)

Absolute structure: Flack x determined using
1883 quotients $[(F^+)-(F^-)]/[(F^+)+(F^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.037 (5)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.70732 (2)	0.68798 (2)	0.59459 (4)	0.01603 (8)
O1	0.76542 (12)	0.78901 (12)	0.77964 (19)	0.0201 (3)
H1O1	0.773 (2)	0.766 (3)	0.881 (2)	0.030*
O2	0.79419 (10)	0.74637 (16)	0.3963 (2)	0.0245 (3)
O3	0.81254 (12)	0.75969 (13)	0.1158 (2)	0.0264 (3)
O4	0.68899 (14)	0.69393 (15)	0.2203 (3)	0.0301 (4)
O5	0.79776 (9)	0.57547 (12)	0.6143 (3)	0.0201 (3)
O6	0.75455 (11)	0.55182 (13)	0.8859 (2)	0.0256 (3)
O7	0.85090 (12)	0.44393 (14)	0.7666 (2)	0.0291 (3)
N1	0.60049 (10)	0.59461 (12)	0.5810 (3)	0.0173 (3)
N2	0.61927 (12)	0.80764 (12)	0.5732 (3)	0.0188 (3)
H2	0.638 (2)	0.856 (2)	0.479 (3)	0.023*
N3	0.76463 (13)	0.73260 (14)	0.2413 (2)	0.0193 (3)
N4	0.80075 (11)	0.52272 (14)	0.7611 (3)	0.0181 (3)
C1	0.59808 (12)	0.48835 (14)	0.6052 (3)	0.0202 (3)
H1	0.652533	0.451412	0.624769	0.024*
C2	0.51962 (13)	0.43077 (14)	0.6027 (4)	0.0236 (3)
H2A	0.520110	0.355445	0.617692	0.028*
C3	0.43973 (14)	0.48534 (17)	0.5779 (3)	0.0267 (4)
H3	0.384490	0.448145	0.578571	0.032*
C4	0.44214 (14)	0.59522 (18)	0.5522 (3)	0.0251 (4)
H4	0.388472	0.634150	0.534687	0.030*
C5	0.52366 (14)	0.64731 (16)	0.5523 (2)	0.0196 (4)
C6	0.53236 (15)	0.76513 (16)	0.5116 (3)	0.0223 (4)
H6A	0.527092	0.776224	0.383523	0.027*
H6AB	0.483274	0.804667	0.569281	0.027*
C7	0.61826 (15)	0.87026 (16)	0.7416 (3)	0.0213 (4)
C8	0.71738 (16)	0.88814 (17)	0.7830 (3)	0.0241 (4)
H8A	0.743334	0.937761	0.695808	0.029*
H8AB	0.723273	0.921226	0.900327	0.029*
C9	0.57393 (18)	0.97932 (19)	0.7166 (3)	0.0307 (5)
H9A	0.603838	1.017915	0.621562	0.046*
H9AB	0.578676	1.020589	0.825375	0.046*
H9AC	0.510874	0.969297	0.686921	0.046*
C10	0.57262 (18)	0.80604 (18)	0.8857 (3)	0.0278 (5)

H10A	0.511114	0.790176	0.850852	0.042*
H10B	0.572316	0.847605	0.994588	0.042*
H10C	0.605093	0.739069	0.904426	0.042*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.01865 (12)	0.01345 (11)	0.01599 (12)	-0.00077 (6)	-0.00037 (10)	0.00057 (10)
O1	0.0285 (8)	0.0172 (6)	0.0146 (6)	-0.0006 (6)	-0.0019 (6)	-0.0012 (5)
O2	0.0284 (8)	0.0316 (8)	0.0136 (7)	-0.0090 (6)	-0.0019 (5)	0.0027 (6)
O3	0.0362 (8)	0.0279 (7)	0.0152 (7)	-0.0099 (6)	0.0022 (7)	0.0028 (6)
O4	0.0301 (9)	0.0375 (10)	0.0226 (8)	-0.0144 (7)	-0.0013 (7)	-0.0045 (6)
O5	0.0222 (6)	0.0196 (6)	0.0184 (8)	0.0025 (4)	0.0013 (6)	0.0035 (6)
O6	0.0281 (8)	0.0301 (7)	0.0185 (7)	0.0043 (6)	0.0045 (6)	0.0005 (6)
O7	0.0355 (9)	0.0255 (7)	0.0263 (7)	0.0120 (6)	0.0004 (7)	0.0058 (6)
N1	0.0183 (6)	0.0162 (6)	0.0174 (7)	-0.0012 (5)	-0.0016 (7)	-0.0004 (7)
N2	0.0242 (7)	0.0156 (6)	0.0167 (9)	0.0008 (5)	0.0001 (7)	0.0010 (6)
N3	0.0264 (8)	0.0160 (7)	0.0154 (7)	-0.0037 (6)	-0.0004 (7)	0.0005 (5)
N4	0.0187 (7)	0.0186 (8)	0.0171 (7)	-0.0013 (5)	-0.0021 (6)	0.0006 (6)
C1	0.0208 (7)	0.0161 (7)	0.0238 (8)	-0.0016 (5)	-0.0048 (9)	0.0012 (8)
C2	0.0247 (8)	0.0204 (7)	0.0256 (8)	-0.0056 (6)	-0.0042 (10)	0.0022 (9)
C3	0.0217 (8)	0.0299 (9)	0.0284 (11)	-0.0072 (7)	-0.0047 (9)	0.0051 (9)
C4	0.0176 (8)	0.0298 (9)	0.0279 (11)	0.0003 (7)	-0.0041 (7)	0.0049 (7)
C5	0.0207 (9)	0.0202 (8)	0.0179 (8)	0.0011 (6)	-0.0026 (6)	0.0028 (6)
C6	0.0247 (10)	0.0205 (9)	0.0217 (9)	0.0023 (7)	-0.0043 (7)	0.0040 (7)
C7	0.0296 (10)	0.0179 (8)	0.0165 (8)	0.0038 (7)	0.0034 (8)	-0.0002 (6)
C8	0.0334 (11)	0.0174 (9)	0.0215 (10)	0.0000 (7)	-0.0005 (8)	-0.0042 (7)
C9	0.0414 (13)	0.0215 (9)	0.0292 (10)	0.0091 (9)	0.0044 (10)	-0.0016 (8)
C10	0.0348 (12)	0.0297 (11)	0.0188 (9)	0.0028 (8)	0.0057 (9)	0.0029 (7)

Geometric parameters (Å, °)

Cu1—O5	1.9608 (14)	C2—C3	1.392 (3)
Cu1—N1	1.9854 (16)	C2—H2A	0.9500
Cu1—N2	2.0033 (17)	C3—C4	1.390 (3)
Cu1—O1	2.0861 (15)	C3—H3	0.9500
Cu1—O2	2.1259 (16)	C4—C5	1.385 (3)
O1—C8	1.435 (3)	C4—H4	0.9500
O1—H10I	0.834 (13)	C5—C6	1.513 (3)
O2—N3	1.274 (2)	C6—H6A	0.9900
O3—N3	1.244 (2)	C6—H6AB	0.9900
O4—N3	1.243 (3)	C7—C10	1.524 (3)
O5—N4	1.301 (3)	C7—C9	1.531 (3)
O6—N4	1.232 (2)	C7—C8	1.535 (3)
O7—N4	1.241 (2)	C8—H8A	0.9900
N1—C1	1.344 (2)	C8—H8AB	0.9900
N1—C5	1.345 (2)	C9—H9A	0.9800
N2—C6	1.484 (3)	C9—H9AB	0.9800

N2—C7	1.505 (3)	C9—H9AC	0.9800
N2—H2	0.977 (13)	C10—H10A	0.9800
C1—C2	1.380 (2)	C10—H10B	0.9800
C1—H1	0.9500	C10—H10C	0.9800
O5—Cu1—N1	97.97 (6)	C2—C3—H3	120.6
O5—Cu1—N2	177.48 (6)	C5—C4—C3	119.3 (2)
N1—Cu1—N2	84.53 (7)	C5—C4—H4	120.4
O5—Cu1—O1	95.45 (7)	C3—C4—H4	120.4
N1—Cu1—O1	136.81 (7)	N1—C5—C4	121.63 (18)
N2—Cu1—O1	82.92 (7)	N1—C5—C6	115.97 (17)
O5—Cu1—O2	83.01 (7)	C4—C5—C6	122.34 (18)
N1—Cu1—O2	131.25 (7)	N2—C6—C5	111.13 (16)
N2—Cu1—O2	95.08 (8)	N2—C6—H6A	109.4
O1—Cu1—O2	91.00 (6)	C5—C6—H6A	109.4
C8—O1—Cu1	109.09 (13)	N2—C6—H6AB	109.4
C8—O1—H10I	111 (3)	C5—C6—H6AB	109.4
Cu1—O1—H10I	118 (3)	H6A—C6—H6AB	108.0
N3—O2—Cu1	113.62 (12)	N2—C7—C10	110.21 (17)
N4—O5—Cu1	117.05 (13)	N2—C7—C9	111.27 (18)
C1—N1—C5	119.01 (16)	C10—C7—C9	111.44 (19)
C1—N1—Cu1	126.70 (13)	N2—C7—C8	104.00 (16)
C5—N1—Cu1	114.22 (13)	C10—C7—C8	111.27 (19)
C6—N2—C7	116.65 (17)	C9—C7—C8	108.41 (19)
C6—N2—Cu1	109.64 (12)	O1—C8—C7	110.84 (17)
C7—N2—Cu1	109.06 (13)	O1—C8—H8A	109.5
C6—N2—H2	103.6 (18)	C7—C8—H8A	109.5
C7—N2—H2	108.1 (19)	O1—C8—H8AB	109.5
Cu1—N2—H2	109.5 (18)	C7—C8—H8AB	109.5
O4—N3—O3	122.21 (18)	H8A—C8—H8AB	108.1
O4—N3—O2	119.33 (18)	C7—C9—H9A	109.5
O3—N3—O2	118.45 (17)	C7—C9—H9AB	109.5
O6—N4—O7	123.36 (19)	H9A—C9—H9AB	109.5
O6—N4—O5	119.70 (17)	C7—C9—H9AC	109.5
O7—N4—O5	116.95 (18)	H9A—C9—H9AC	109.5
N1—C1—C2	122.58 (17)	H9AB—C9—H9AC	109.5
N1—C1—H1	118.7	C7—C10—H10A	109.5
C2—C1—H1	118.7	C7—C10—H10B	109.5
C1—C2—C3	118.62 (17)	H10A—C10—H10B	109.5
C1—C2—H2A	120.7	C7—C10—H10C	109.5
C3—C2—H2A	120.7	H10A—C10—H10C	109.5
C4—C3—C2	118.86 (18)	H10B—C10—H10C	109.5
C4—C3—H3	120.6		
Cu1—O2—N3—O4	4.0 (3)	C7—N2—C6—C5	-101.79 (19)
Cu1—O2—N3—O3	-176.76 (14)	Cu1—N2—C6—C5	22.8 (2)
Cu1—O5—N4—O6	-7.5 (2)	N1—C5—C6—N2	-20.6 (2)
Cu1—O5—N4—O7	172.10 (14)	C4—C5—C6—N2	162.32 (19)

C5—N1—C1—C2	-0.4 (4)	C6—N2—C7—C10	52.6 (2)
Cu1—N1—C1—C2	176.29 (18)	Cu1—N2—C7—C10	-72.26 (19)
N1—C1—C2—C3	-1.4 (4)	C6—N2—C7—C9	-71.6 (2)
C1—C2—C3—C4	1.6 (4)	Cu1—N2—C7—C9	163.60 (15)
C2—C3—C4—C5	-0.1 (4)	C6—N2—C7—C8	171.93 (16)
C1—N1—C5—C4	1.9 (3)	Cu1—N2—C7—C8	47.09 (17)
Cu1—N1—C5—C4	-175.13 (15)	Cu1—O1—C8—C7	32.1 (2)
C1—N1—C5—C6	-175.2 (2)	N2—C7—C8—O1	-52.1 (2)
Cu1—N1—C5—C6	7.7 (2)	C10—C7—C8—O1	66.5 (2)
C3—C4—C5—N1	-1.7 (3)	C9—C7—C8—O1	-170.60 (18)
C3—C4—C5—C6	175.3 (2)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O1—H1O1 \cdots O3 ⁱ	0.83 (1)	1.89 (2)	2.685 (2)	159 (4)
N2—H2 \cdots O7 ⁱⁱ	0.98 (1)	1.97 (2)	2.930 (3)	167 (3)
C4—H4 \cdots O2 ⁱⁱⁱ	0.95	2.31	3.204 (3)	156
C8—H8 AB \cdots O5 ^{iv}	0.99	2.55	3.455 (3)	152

Symmetry codes: (i) $x, y, z+1$; (ii) $-x+3/2, y+1/2, z-1/2$; (iii) $x-1/2, -y+3/2, z$; (iv) $-x+3/2, y+1/2, z+1/2$.