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[μ-*N*,*N*,*N*′,*N*′-Tetrakis(pyridin-2-ylmethyl)butane-1,4-diamine]bis[(dimethanol-κO)(perchlorato-κO)-copper(II)] bis(perchlorate)

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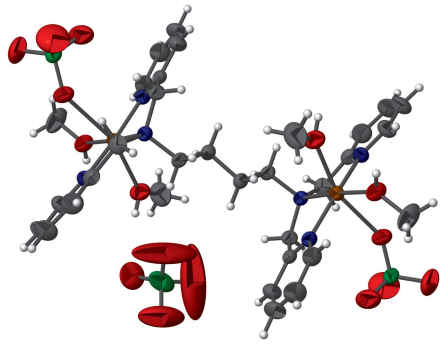
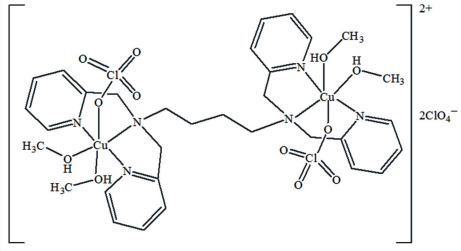
Structural data: full structural data are available from iucrdata.iucr.org

The binuclear cation of the title compound, $[Cu_2(ClO_4)_2(C_{28}H_{32}N_6)(CH_3OH)_4](ClO_4)_2$, is located on an inversion centre. The Cu^{II} atom adopts a distorted octahedral coordination geometry due to the Jahn–Teller effect. The equatorial plane consists of one methanol molecule and three N atoms from the *N*,*N*,*N*′,*N*′-tetrakis(pyridin-2-ylmethyl)butane-1,4-diamine ligand. The Cu—N bond lengths are in the range 1.975 (3)–2.041 (2) Å and the Cu—O bond length is 2.008 (2) Å. The axial coordination sites of the Cu^{II} atom are occupied by the O atoms of one methanol molecule and one perchlorate anion, with Cu—O bond lengths of 2.385 (3) and 2.565 (3) Å, respectively. In the crystal, the cations and the perchlorate anions are connected *via* O—H···O hydrogen bonds. In addition, weak C—H···O interactions stabilize the structure.

3D view



Chemical scheme



Structure description

Transition metal complexes of tetrakis(pyridin-2-yl-methyl)alkyldiamine ligands have attracted much attention recently (Mambanda *et al.*, 2010; Bartholomä *et al.*, 2009). We report herein the crystal structure of the title complex $[Cu_2(ClO_4)_2(C_{28}H_{32}N_6)(CH_3OH)_4](ClO_4)_2$ (Fig. 1).

Crystal structures of some dicopper(II) and dicadmium(II) complexes closely related to the title compound have been reported (Bartholomä *et al.*, 2010*a*,*b*,*c*,*d*,*e*; Tahsini *et al.*, 2012). The copper(II) atoms in the previously reported dicopper(II) complexes adopt a distorted square-pyramidal or a pseudotetrahedral coordination geometry. Polymeric

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···O7^{i}	0.83 (1)	2.01 (2)	2.819 (4)	163 (4)
O1—H1A···O10	0.84 (1)	2.76 (5)	3.340 (7)	128 (5)
O1—H1A···O7	0.84 (1)	2.28 (2)	3.102 (5)	169 (6)
C2—H2···O10^{ii}	0.93	2.52	3.189 (7)	129
C4—H4···O8^{iii}	0.93	2.55	3.153 (7)	123
C13—H13B···O5^{iv}	0.96	2.56	3.325 (5)	136
C15—H15A···O10	0.97	2.38	3.326 (5)	166

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

coordination compounds based on copper complexes of diamine ligands have been synthesized (Bartholomä *et al.*, 2011; Khullar & Mandal, 2014). The oxygen reduction reaction activity of copper complexes of diamine ligands has also been studied (Tse *et al.*, 2014).

In the crystal, the cations and the perchlorate anions are connected *via* O—H···O hydrogen bonds (Table 1). In addition, weak C—H···O interactions stabilize the structure. These interactions give rise to a two-dimensional network parallel to (101).

Synthesis and crystallization

The ligand μ-*N,N,N′,N′*-tetrakis(pyrid-2-ylmethyl)butane-1,4-diamine (45.3 mg, 0.10 mmol) was dissolved in 10 ml CH_3OH to form a clear solution, to which was added a CH_3OH solution (6 ml) of $Cu(ClO_4)_2{\cdot}6H_2O$ (74.1 mg, 0.20 mmol). The solution turned deep blue immediately and a small amount of precipitate appeared. The mixture was stirred at room temperature for 24 h. A cloudy blue solution was obtained and filtered. The filtrate was diffused by diethyl ether and blue block-shaped crystals were obtained after one week. Yield: 83 mg (75%). Analysis found: C, 34.57; H. 4.24; N, 7.45. Calculated for $C_{32}H_{48}Cl_4Cu_2N_6O_{20}$: C, 34.76; H, 4.38; N, 7.60%. IR (KBr pellet, cm^{-1}): 3432, 3033, 2911, 2856, 1614, 1418, 1083 (*vs*), 771, 637.

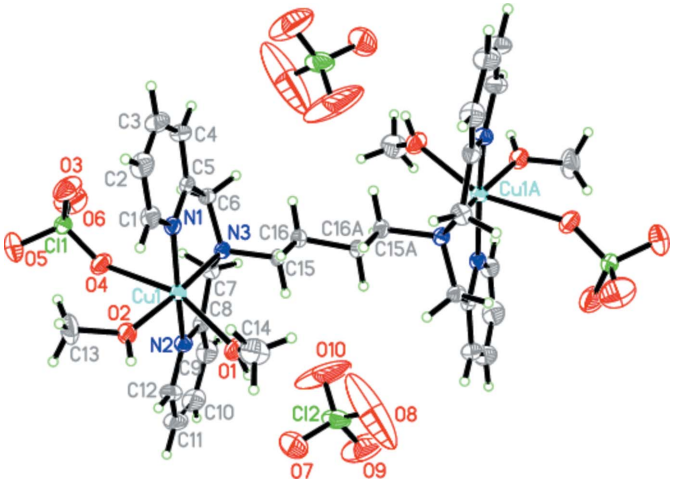


Figure 1
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (A) $-x, -y+1, -z+1$.]

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Cu_2(ClO_4)_2(C_{28}H_{32}N_6)(CH_4O)_4]$-$(ClO_4)_2$
M_r	1105.64
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	296
a, b, c (Å)	15.262 (6), 9.355 (4), 15.832 (6)
β (°)	92.858 (4)
V (Å^3)	2257.6 (16)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.26
Crystal size (mm)	0.15 × 0.12 × 0.10
Data collection	
Diffractometer	Siemens SMART CCD area-detector
Absorption correction	Multi-scan (*SADABS*; Sheldrick,1996)
T_{min}, T_{max}	0.833, 0.884
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10866, 4092, 3585
R_{int}	0.022
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.602
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.119, 1.05
No. of reflections	4092
No. of parameters	299
No. of restraints	22
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.96, −0.51

Computer programs: *SMART* (Siemens, 1996), *SAINT* (Siemens, 1996), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *SHELXTL* (Sheldrick, 2008).

Refinement

Crystal data, data collection, and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

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Crystal data

$[Cu_2(ClO_4)_2(C_{28}H_{32}N_6)(CH_4O)_4](ClO_4)_2$
M_r = 1105.64
Monoclinic, $P2_1/n$
a = 15.262 (6) Å
b = 9.355 (4) Å
c = 15.832 (6) Å
β = 92.858 (4)°
V = 2257.6 (16) Å^3
Z = 2
$F(000)$ = 1136
D_x = 1.626 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 10866 reflections
θ = 2.5–25.4°
μ = 1.26 mm^{-1}
T = 296 K
Cuboid, blue
0.15 × 0.12 × 0.10 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick,1996)
T_{min} = 0.833, T_{max} = 0.884
10866 measured reflections
4092 independent reflections
3585 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 25.4°, θ_{min} = 2.5°
h = −18→18
k = −10→11
l = −19→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.119
S = 1.05
4092 reflections
299 parameters
22 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0693P)^2 + 2.3032P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.96 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.1455 (2)	0.0368 (3)	0.5044 (2)	0.0440 (8)
H1	0.1648	0.0170	0.4509	0.053*
C2	0.0999 (3)	−0.0655 (4)	0.5452 (3)	0.0620 (11)
H2	0.0883	−0.1536	0.5197	0.074*
C3	0.0714 (3)	−0.0365 (4)	0.6244 (3)	0.0644 (11)
H3	0.0414	−0.1058	0.6537	0.077*
C4	0.0875 (2)	0.0954 (4)	0.6600 (2)	0.0505 (9)
H4	0.0671	0.1177	0.7127	0.061*
C5	0.13469 (18)	0.1947 (3)	0.61593 (19)	0.0344 (7)
C6	0.1599 (2)	0.3373 (3)	0.65356 (18)	0.0358 (7)
H6A	0.1100	0.3784	0.6805	0.043*
H6B	0.2069	0.3246	0.6964	0.043*
C7	0.2619 (2)	0.5306 (4)	0.6191 (2)	0.0391 (7)
H7A	0.2967	0.4812	0.6629	0.047*
H7B	0.2378	0.6160	0.6437	0.047*
C8	0.31903 (19)	0.5715 (3)	0.5488 (2)	0.0368 (7)
C9	0.3711 (3)	0.6939 (4)	0.5513 (3)	0.0555 (10)
H9	0.3684	0.7588	0.5956	0.067*
C10	0.4271 (3)	0.7166 (5)	0.4864 (3)	0.0673 (12)
H10	0.4634	0.7964	0.4872	0.081*
C11	0.4287 (3)	0.6211 (5)	0.4211 (3)	0.0628 (11)
H11	0.4660	0.6357	0.3772	0.075*
C12	0.3750 (2)	0.5037 (4)	0.4209 (2)	0.0490 (8)
H12	0.3754	0.4400	0.3758	0.059*
C13	0.3553 (3)	0.0668 (5)	0.4236 (3)	0.0731 (13)
H13A	0.3653	0.0485	0.4829	0.110*
H13B	0.4099	0.0895	0.3992	0.110*
H13C	0.3302	−0.0165	0.3965	0.110*
C14	0.1120 (3)	0.3258 (6)	0.3058 (3)	0.0769 (14)
H14A	0.1070	0.2258	0.3182	0.115*
H14B	0.1309	0.3376	0.2493	0.115*
H14C	0.0561	0.3712	0.3107	0.115*
C15	0.11512 (18)	0.5284 (3)	0.55231 (19)	0.0325 (6)
H15A	0.1368	0.5876	0.5076	0.039*
H15B	0.0972	0.5917	0.5968	0.039*
C16	0.03470 (18)	0.4473 (3)	0.51735 (19)	0.0343 (6)
H16A	0.0107	0.3901	0.5618	0.041*
H16B	0.0513	0.3834	0.4726	0.041*
Cl1	0.37875 (5)	0.12281 (9)	0.66713 (5)	0.0410 (2)
Cl2	0.15310 (9)	0.76483 (12)	0.30737 (7)	0.0715 (3)
Cu1	0.24114 (2)	0.31381 (4)	0.49533 (2)	0.02964 (14)
N1	0.16344 (16)	0.1652 (3)	0.53909 (16)	0.0329 (5)
N2	0.32171 (15)	0.4784 (3)	0.48422 (16)	0.0357 (6)
N3	0.18915 (14)	0.4362 (3)	0.58710 (14)	0.0294 (5)
O1	0.17400 (17)	0.3889 (3)	0.36349 (16)	0.0527 (6)

H1A	0.190 (4)	0.465 (4)	0.342 (4)	0.12 (2)*
O2	0.29635 (17)	0.1842 (3)	0.41199 (15)	0.0472 (6)
H2A	0.287 (3)	0.194 (4)	0.3599 (8)	0.057 (12)*
O3	0.3075 (2)	0.0238 (4)	0.6663 (2)	0.0861 (11)
O4	0.36000 (16)	0.2327 (3)	0.60525 (16)	0.0563 (7)
O5	0.4561 (2)	0.0499 (4)	0.6471 (2)	0.0976 (12)
O6	0.3892 (3)	0.1839 (4)	0.7486 (2)	0.1032 (13)
O7	0.2095 (3)	0.6690 (4)	0.2660 (2)	0.0938 (11)
O8	0.0697 (4)	0.7308 (12)	0.2688 (9)	0.373 (10)
O9	0.1657 (5)	0.9069 (4)	0.2901 (3)	0.169 (3)
O10	0.1527 (8)	0.7413 (7)	0.3898 (3)	0.286 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0466 (17)	0.0288 (16)	0.056 (2)	−0.0009 (14)	0.0012 (15)	−0.0048 (14)
C2	0.063 (2)	0.0303 (19)	0.093 (3)	−0.0080 (17)	0.003 (2)	0.0013 (19)
C3	0.059 (2)	0.045 (2)	0.090 (3)	−0.0126 (18)	0.013 (2)	0.024 (2)
C4	0.0485 (19)	0.051 (2)	0.053 (2)	−0.0015 (16)	0.0116 (15)	0.0169 (17)
C5	0.0295 (14)	0.0351 (16)	0.0387 (16)	0.0057 (12)	0.0015 (12)	0.0104 (12)
C6	0.0405 (16)	0.0399 (17)	0.0273 (15)	0.0044 (13)	0.0046 (12)	0.0033 (12)
C7	0.0389 (15)	0.0385 (17)	0.0393 (17)	−0.0040 (13)	−0.0028 (13)	−0.0097 (13)
C8	0.0345 (15)	0.0308 (16)	0.0444 (17)	−0.0011 (12)	−0.0059 (12)	0.0012 (13)
C9	0.056 (2)	0.038 (2)	0.072 (3)	−0.0118 (16)	−0.0053 (19)	−0.0039 (17)
C10	0.057 (2)	0.050 (2)	0.095 (3)	−0.0224 (19)	0.000 (2)	0.017 (2)
C11	0.056 (2)	0.064 (3)	0.069 (3)	−0.016 (2)	0.0145 (19)	0.020 (2)
C12	0.0479 (18)	0.056 (2)	0.0436 (19)	−0.0082 (17)	0.0092 (14)	0.0059 (16)
C13	0.078 (3)	0.076 (3)	0.064 (3)	0.043 (2)	−0.003 (2)	−0.017 (2)
C14	0.057 (2)	0.118 (4)	0.055 (3)	−0.019 (3)	−0.0119 (19)	−0.001 (2)
C15	0.0348 (14)	0.0268 (15)	0.0358 (15)	0.0064 (12)	0.0021 (12)	0.0015 (11)
C16	0.0325 (14)	0.0317 (16)	0.0387 (16)	0.0053 (12)	0.0031 (12)	0.0026 (12)
Cl1	0.0359 (4)	0.0506 (5)	0.0363 (4)	0.0061 (3)	−0.0019 (3)	0.0082 (3)
Cl2	0.0999 (8)	0.0561 (6)	0.0623 (6)	−0.0027 (6)	0.0418 (6)	−0.0047 (5)
Cu1	0.0313 (2)	0.0263 (2)	0.0317 (2)	−0.00060 (13)	0.00539 (14)	−0.00210 (13)
N1	0.0324 (12)	0.0268 (13)	0.0395 (14)	0.0013 (10)	0.0012 (10)	0.0017 (10)
N2	0.0330 (12)	0.0357 (14)	0.0384 (14)	−0.0037 (10)	0.0016 (10)	0.0039 (11)
N3	0.0314 (12)	0.0275 (12)	0.0293 (12)	0.0012 (10)	0.0002 (9)	−0.0011 (9)
O1	0.0553 (15)	0.0547 (17)	0.0468 (14)	−0.0034 (13)	−0.0105 (11)	0.0086 (12)
O2	0.0603 (15)	0.0469 (14)	0.0348 (13)	0.0181 (11)	0.0072 (11)	−0.0012 (10)
O3	0.0678 (18)	0.082 (2)	0.106 (3)	−0.0239 (17)	−0.0199 (17)	0.043 (2)
O4	0.0545 (15)	0.0567 (16)	0.0568 (15)	0.0015 (12)	−0.0068 (12)	0.0217 (13)
O5	0.0637 (19)	0.109 (3)	0.122 (3)	0.046 (2)	0.0188 (19)	0.022 (2)
O6	0.139 (3)	0.125 (3)	0.0444 (18)	−0.008 (3)	−0.0083 (19)	−0.0154 (18)
O7	0.098 (3)	0.106 (3)	0.080 (2)	0.018 (2)	0.027 (2)	−0.013 (2)
O8	0.111 (5)	0.333 (13)	0.68 (2)	0.000 (7)	0.087 (9)	−0.317 (16)
O9	0.310 (8)	0.074 (3)	0.128 (4)	0.013 (4)	0.067 (5)	0.035 (3)
O10	0.661 (19)	0.120 (4)	0.095 (4)	0.099 (8)	0.187 (7)	0.044 (3)

Geometric parameters (Å, º)

C1—N1	1.343 (4)	C13—H13B	0.9600
C1—C2	1.364 (5)	C13—H13C	0.9600
C1—H1	0.9300	C14—O1	1.411 (5)
C2—C3	1.375 (6)	C14—H14A	0.9600
C2—H2	0.9300	C14—H14B	0.9600
C3—C4	1.374 (6)	C14—H14C	0.9600
C3—H3	0.9300	C15—N3	1.504 (3)
C4—C5	1.385 (4)	C15—C16	1.524 (4)
C4—H4	0.9300	C15—H15A	0.9700
C5—N1	1.342 (4)	C15—H15B	0.9700
C5—C6	1.503 (4)	C16—C16^{i}	1.529 (5)
C6—N3	1.486 (4)	C16—H16A	0.9700
C6—H6A	0.9700	C16—H16B	0.9700
C6—H6B	0.9700	Cl1—O6	1.412 (3)
C7—N3	1.487 (4)	Cl1—O5	1.413 (3)
C7—C8	1.498 (4)	Cl1—O3	1.427 (3)
C7—H7A	0.9700	Cl1—O4	1.439 (2)
C7—H7B	0.9700	Cl2—O10	1.323 (4)
C8—N2	1.344 (4)	Cl2—O9	1.372 (4)
C8—C9	1.393 (5)	Cl2—O8	1.419 (6)
C9—C10	1.385 (6)	Cl2—O7	1.424 (3)
C9—H9	0.9300	Cu1—N1	1.975 (3)
C10—C11	1.367 (7)	Cu1—N2	1.984 (3)
C10—H10	0.9300	Cu1—O2	2.008 (2)
C11—C12	1.371 (5)	Cu1—N3	2.041 (2)
C11—H11	0.9300	Cu1—O1	2.385 (3)
C12—N2	1.342 (4)	Cu1—O4	2.565 (3)
C12—H12	0.9300	O1—H1A	0.835 (10)
C13—O2	1.425 (4)	O2—H2A	0.834 (10)
C13—H13A	0.9600		

N1—C1—C2	122.2 (4)	H14B—C14—H14C	109.5
N1—C1—H1	118.9	N3—C15—C16	115.1 (2)
C2—C1—H1	118.9	N3—C15—H15A	108.5
C1—C2—C3	119.0 (4)	C16—C15—H15A	108.5
C1—C2—H2	120.5	N3—C15—H15B	108.5
C3—C2—H2	120.5	C16—C15—H15B	108.5
C4—C3—C2	119.5 (3)	H15A—C15—H15B	107.5
C4—C3—H3	120.2	C15—C16—C16^{i}	109.9 (3)
C2—C3—H3	120.2	C15—C16—H16A	109.7
C3—C4—C5	118.9 (4)	C16^{i}—C16—H16A	109.7
C3—C4—H4	120.5	C15—C16—H16B	109.7
C5—C4—H4	120.5	C16^{i}—C16—H16B	109.7
N1—C5—C4	121.3 (3)	H16A—C16—H16B	108.2
N1—C5—C6	116.9 (3)	O6—Cl1—O5	110.0 (3)
C4—C5—C6	121.7 (3)	O6—Cl1—O3	108.8 (2)

N3—C6—C5	110.6 (2)	O5—Cl1—O3	109.2 (2)
N3—C6—H6A	109.5	O6—Cl1—O4	110.0 (2)
C5—C6—H6A	109.5	O5—Cl1—O4	109.4 (2)
N3—C6—H6B	109.5	O3—Cl1—O4	109.37 (17)
C5—C6—H6B	109.5	O10—Cl2—O9	111.4 (4)
H6A—C6—H6B	108.1	O10—Cl2—O8	109.8 (7)
N3—C7—C8	110.6 (2)	O9—Cl2—O8	105.3 (6)
N3—C7—H7A	109.5	O10—Cl2—O7	112.4 (4)
C8—C7—H7A	109.5	O9—Cl2—O7	115.1 (3)
N3—C7—H7B	109.5	O8—Cl2—O7	102.2 (3)
C8—C7—H7B	109.5	N1—Cu1—N2	164.38 (11)
H7A—C7—H7B	108.1	N1—Cu1—O2	94.85 (11)
N2—C8—C9	121.0 (3)	N2—Cu1—O2	97.37 (11)
N2—C8—C7	116.1 (3)	N1—Cu1—N3	83.31 (10)
C9—C8—C7	122.7 (3)	N2—Cu1—N3	83.82 (10)
C10—C9—C8	118.4 (4)	O2—Cu1—N3	175.70 (9)
C10—C9—H9	120.8	N1—Cu1—O1	105.97 (10)
C8—C9—H9	120.8	N2—Cu1—O1	86.27 (10)
C11—C10—C9	119.7 (4)	O2—Cu1—O1	77.22 (10)
C11—C10—H10	120.1	N3—Cu1—O1	107.01 (10)
C9—C10—H10	120.1	C5—N1—C1	119.0 (3)
C10—C11—C12	119.5 (4)	C5—N1—Cu1	113.7 (2)
C10—C11—H11	120.3	C1—N1—Cu1	126.9 (2)
C12—C11—H11	120.3	C12—N2—C8	119.7 (3)
N2—C12—C11	121.6 (4)	C12—N2—Cu1	127.2 (2)
N2—C12—H12	119.2	C8—N2—Cu1	113.1 (2)
C11—C12—H12	119.2	C6—N3—C7	112.0 (2)
O2—C13—H13A	109.5	C6—N3—C15	111.7 (2)
O2—C13—H13B	109.5	C7—N3—C15	108.6 (2)
H13A—C13—H13B	109.5	C6—N3—Cu1	107.21 (18)
O2—C13—H13C	109.5	C7—N3—Cu1	105.37 (17)
H13A—C13—H13C	109.5	C15—N3—Cu1	111.88 (17)
H13B—C13—H13C	109.5	C14—O1—Cu1	133.5 (3)
O1—C14—H14A	109.5	C14—O1—H1A	107 (4)
O1—C14—H14B	109.5	Cu1—O1—H1A	119 (4)
H14A—C14—H14B	109.5	C13—O2—Cu1	131.6 (2)
O1—C14—H14C	109.5	C13—O2—H2A	106 (3)
H14A—C14—H14C	109.5	Cu1—O2—H2A	122 (3)

N1—C1—C2—C3	−0.1 (6)	C6—C5—N1—Cu1	4.2 (3)
C1—C2—C3—C4	1.5 (6)	C2—C1—N1—C5	−0.8 (5)
C2—C3—C4—C5	−2.0 (6)	C2—C1—N1—Cu1	171.4 (3)
C3—C4—C5—N1	1.1 (5)	C11—C12—N2—C8	1.5 (5)
C3—C4—C5—C6	−175.8 (3)	C11—C12—N2—Cu1	−179.1 (3)
N1—C5—C6—N3	17.5 (3)	C9—C8—N2—C12	−0.4 (5)
C4—C5—C6—N3	−165.5 (3)	C7—C8—N2—C12	−176.5 (3)
N3—C7—C8—N2	−27.3 (4)	C9—C8—N2—Cu1	−179.8 (3)
N3—C7—C8—C9	156.7 (3)	C7—C8—N2—Cu1	4.1 (3)

N2—C8—C9—C10	−1.0 (5)	C5—C6—N3—C7	−144.0 (2)
C7—C8—C9—C10	174.9 (3)	C5—C6—N3—C15	94.0 (3)
C8—C9—C10—C11	1.3 (6)	C5—C6—N3—Cu1	−28.9 (3)
C9—C10—C11—C12	−0.2 (7)	C8—C7—N3—C6	151.1 (2)
C10—C11—C12—N2	−1.3 (6)	C8—C7—N3—C15	−85.1 (3)
N3—C15—C16—C16^{i}	−179.0 (3)	C8—C7—N3—Cu1	34.9 (3)
C4—C5—N1—C1	0.3 (4)	C16—C15—N3—C6	−55.7 (3)
C6—C5—N1—C1	177.3 (3)	C16—C15—N3—C7	−179.6 (2)
C4—C5—N1—Cu1	−172.9 (2)	C16—C15—N3—Cu1	64.5 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*A*···O7^{ii}	0.83 (1)	2.01 (2)	2.819 (4)	163 (4)
O1—H1*A*···O10	0.84 (1)	2.76 (5)	3.340 (7)	128 (5)
O1—H1*A*···O7	0.84 (1)	2.28 (2)	3.102 (5)	169 (6)
C2—H2···O10^{iii}	0.93	2.52	3.189 (7)	129
C4—H4···O8^{i}	0.93	2.55	3.153 (7)	123
C13—H13*B*···O5^{iv}	0.96	2.56	3.325 (5)	136
C15—H15*A*···O10	0.97	2.38	3.326 (5)	166

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