metal-organic compounds

(5,16-Dimethyl-2,6,13,17-tetraaza-tricyclo[14.4.0^{1,18}.0^{7,12}]docosane-$\kappa^4 N$)-bis(perchlorato-κO)copper(II)

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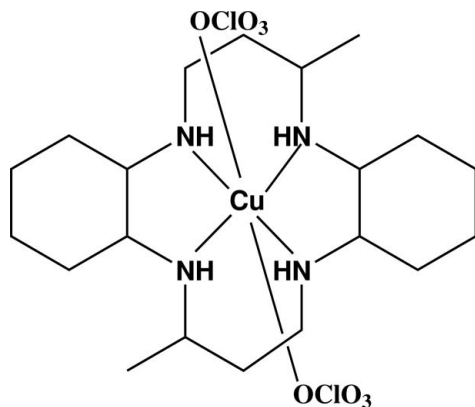
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In the title compound, [Cu(ClO$_4$)$_2$(C$_{20}$H$_{40}$N$_4$)], the Cu^{II} ion has a tetragonally distorted octahedral environment, with the four N atoms of the macrocyclic ligand in equatorial positions and the O atoms of two perchlorate groups in axial positions. The Cu^{II} ion is situated on an inversion centre. The macrocyclic ligand adopts its most stable *trans*-III conformation. The long axial Cu—O bond is the result of the Jahn–Teller effect. The crystal structure is stabilized by intramolecular hydrogen bonds between secondary N—H and the O atoms of the perchlorate groups.

Related literature

For related literature, see: Bakaj & Zimmer (1999); Choi *et al.* (1996); Choi, Clegg *et al.* (2006); Choi, Suzuki & Kaizaki (2006); Kang *et al.* (1991); Karunakaran *et al.* (1999); Liang & Sadler (2004); Meyer *et al.* (1998); Nakamoto (1997).

Experimental

Crystal data

[Cu(ClO$_4$)$_2$(C$_{20}$H$_{40}$N$_4$)]	V = 2571.5 (3) Å^3
M_r = 599.00	Z = 4
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
a = 18.8782 (12) Å	μ = 1.11 mm^{-1}
b = 8.0923 (5) Å	T = 173 (2) K
c = 16.8906 (11) Å	0.40 × 0.30 × 0.20 mm
β = 94.741 (1)°	

Data collection

Bruker SMART CCD area-detector diffractometer	7765 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1999)	2914 independent reflections
T_{min} = 0.222, T_{max} = 0.288	2627 reflections with $I > 2\sigma(I)$
(expected range = 0.617–0.801)	R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.103	
S = 1.26	
2914 reflections	$\Delta\rho_{max}$ = 0.52 e Å^{-3}
168 parameters	$\Delta\rho_{min}$ = −1.02 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N2	2.005 (2)	Cu1—O4	2.623 (2)
Cu1—N1	2.048 (2)		
N2—Cu1—N1	85.04 (9)	N1—Cu1—O4	84.11 (9)
N2—Cu1—O4	86.65 (9)		

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$\cdots$O1	0.85 (3)	2.28 (3)	3.110 (4)	166 (2)
N2—H2$\cdots$O3^i	0.77 (3)	2.34 (3)	3.084 (4)	162 (3)

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AV3109).

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supplementary materials

(5,16-Dimethyl-2,6,13,17-tetraazatricyclo[14.4.0^{1,18}.0^{7,12}]docosane-κ^{4}N)bis(perchlorato-κO)copper(II)

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Comment

Marcrocyclic complexes are involved in diverse application fields such as catalysis, enzyme mimics, chemical sensors, purification of waste water, selective metal ions recovery, pharmacology and therapy (Meyer *et al.*, 1998, and references therein). Recently, metal-containing complexes of 14-membered cyclam and its derivatives have received a great deal of attention due to their highly potent and selective *anti*-HIV activity by specifically blocking the co-receptor CXCR4. It is found that the transition metal complexation to the cyclam ligands shows various antiviral activity in comparison to the marcrocycles alone (Liang & Sadler, 2004).

There are five configurational *trans* isomers of metal–cyclam complexes, which differ in the chirality of the N atoms. The configurations that are symmetrical about the diagonal also can fold to form *cis* isomers. The substitution on the ring of cyclam derivatives has a very important effect both on the chemical and the structural properties of complexes containing the macrocyclic ligands (Bakaj & Zimmer, 1999).

The crystal structures of copper(II) complexes containing ligand 5,16-dimethyl-2,6,13,17-tetraazatricyclo(14,4,0$^{1.18}$,0$^{7.12}$)docosane (*L*) have been reported previously (Choi *et al.*, 1996; Choi, Suzuki & Kaizaki, 2006). The constrained ligand **L** containing two cyclohexane rings and methyl groups on the carbon atoms has often shown different coordination behaviors from those of the transition metal complexes with the cyclam.

The perchlorate ion, ClO$_4^-$ also can coordinate to the transition metal ions as monodentate, chelating bidentate, and bridging bidentate ligand (Nakamoto, 1997).

The configuration of the macrocyclic ligand and orientation of the N—H bonds in the metal complexes are important factors for co-receptor recognition. Therefore, the understanding of binding affinity and configuration between perchlorato group and copper(II)-constrained cyclam has become extremely important in the improved design and development of new highly effective *anti*-HIV drugs that specially target alternative events in the HIV replicative cycle.

In this communication, we report the structure of the copper(II) complex, (I), with the 14-membered macrocycle (*L*) and perchlorato groups in order to determine the coordination mode of perchlorato group and the macrocyclic ring conformation.

The selected bond lengths and angles are listed in Table 1. A perspective drawing of the structure together with the atomic labeling is depicted in Fig. 1.

The coordination geometry around the copper(II) ion reveals a tetragonally distorted coordination environment with four N atoms from the macrocycle and two O atoms atoms of the perchlorato groups. The copper ion is situated on the centre of inversion. Two methyl groups on the six-membered chelate rings are *anti* with respect to the N$_4$ plane. As usually observed, five-membered chelate rings adopt a *gauche*, and six-membered rings are in the chair conformations. The bond

angles of five- and six-membered chelate rings around the copper(II) are the 85.04 (9) and 94.96 (9)°, respectively. The C—N and C—C distances in macrocyclic molecule are typical of macrocyclic tetramine complexes, 1.490 (3)–1.500 (3) Å and 1.517 (4)–1.533 (4) Å, respectively. The C—N—C and C—C—N angles are also typical (Choi, Clegg *et al.*, 2006). The equatorial Cu—N1 [2.048 (2) Å] and Cu—N2 [2.005 (2) Å] bond distances are slightly different due to steric effect of the methyl group attached to the C9, and can be compared to corresponding bond lengths in other tetragonally elongated octahedral copper(II) complexes. However, the average bond length [2.027 Å] of Cu—N is in good agreement with those [2.028 Å and 2.025 Å] found in [Cu(*L*)(H$_2$O)$_2$]Cl$_2$ and [Cu(*L*)(ONO$_2$)$_2$]·3H$_2$O, respectively (Choi *et al.*, 1996; Choi, Suzuki & Kaizaki, 2006). In general, the Cu(II)–ligand bonds in the range of 2.5 and 2.9 Å may be considered as semi-coordinated bond (Karunakaran *et al.*, 1999). The Cu1—O4 bond length of 2.623 (2) Å is the result of the Jahn–Teller effect. The Cl—O bond lengths in the perchlorate anion are in the range 1.419 (2)–1.442 (3) Å. The longer Cl1—O4 bond reflects that the O atom of perchlorato group is coordinated to the copper atom. The Cl1—O1 and Cl1—O3 bonds are slightly longer than Cl1—O2 bond, and the O—Cl—O angle deviating from the ideal value of 109° involves the O1 and O3 atoms linked to the cation by hydrogen bonds N1—H1⋯O1 and N2—H2⋯O3A. Thus the complex is stabilized by formation of the intramolecular hydrogen bond between the non-coordinated oxygen O1 and O3 of the perchlorato ligand and the secondary NH group of the macrocyclic ligand (Table 2).

Experimental

The macrocyclicligand 5,16-dimethyl-2,6,13,17-tetraazatricyclo[14,4,0$^{1.18}$,0$^{7.12}$]docosane (*L*) was prepared according to the literature method (Kang *et al.*, 1991). A methanol suspension of Cu(OAc)·H$_2$O (0.95 g, 2.10 mmol) and the macrocyclic ligand (*L*) (1.0 g, 3 mmol) was heated to reflux for 30 min. The suspension mixture is refluxed for 30 min at 80 °C and cooled to room temperature. The HClO$_4$ (60%, 0.66 ml) is added the reaction mixture and the solution is stored in the refrigerator. The product was filtered and air-dried. Recrystallization of the material from hot acetonitrile–water (1:2 *v/v*) mixture solution gave reddish violet crystals that were suitable for crystallographic analysis. Analysis calculated for C$_{20}$H$_{48}$Cl$_2$CuN$_4$O$_8$: C, 40.10; H, 6.73; N, 9.35%; found: C, 40.15; H, 6.94; N, 9.31%.

Refinement

The hydrogen atoms (H1 and H2) attached to nitrogen atoms were located in difference electron density maps, and refined isotropically. All the other hydrogen atoms were included in calculated positions and refined using a riding model, with C—H = 0.96–0.98 Å and with U_{iso}(H) = 1.2 (1.5 for methyl groups) times U_{eq}(parent atom).
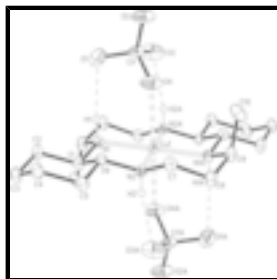
Figures

Fig. 1. A perspective view (50% probability level) of complex (I) with the atom-numbering scheme. Dashed lines indicate intramolecular hydrogen bonds.

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Crystal data

[Cu(ClO$_4$)$_2$(C$_{20}$H$_{40}$N$_4$)]	F_{000} = 1260
M_r = 599.00	D_x = 1.547 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 4468 reflections
a = 18.8782 (12) Å	θ = 2.2–28.2º
b = 8.0923 (5) Å	μ = 1.11 mm^{-1}
c = 16.8906 (11) Å	*T* = 173 (2) K
β = 94.7410 (10)º	Block, red-violet
V = 2571.5 (3) Å^3	0.40 × 0.30 × 0.20 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	2914 independent reflections
Radiation source: fine-focus sealed tube	2627 reflections with $I > 2σ(I)$
Monochromator: graphite	R_{int} = 0.026
T = 173(2) K	$θ_{max}$ = 27.5º
φ and ω scans	$θ_{min}$ = 2.2º
Absorption correction: multi-scan (SADABS; Sheldrick, 1999)	*h* = −24→24
T_{min} = 0.222, T_{max} = 0.288	*k* = −9→10
7765 measured reflections	*l* = −21→20

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2σ(F^2)]$ = 0.051	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.103	$w = 1/[σ^2(F_o^2) + (0.0275P)^2 + 8.4134P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.26	$(Δ/σ)_{max}$ = 0.001
2914 reflections	$Δρ_{max}$ = 0.52 e Å^{-3}
168 parameters	$Δρ_{min}$ = −1.02 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

supplementary materials

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	$U_{iso}*/U_{eq}$
Cu1	0.5000	0.5000	0.5000	0.01430 (13)
Cl1	0.59889 (4)	0.27519 (9)	0.36069 (5)	0.02685 (18)
O1	0.66514 (14)	0.3277 (4)	0.4016 (2)	0.0628 (9)
O2	0.60819 (15)	0.1267 (3)	0.31806 (16)	0.0448 (7)
O3	0.57461 (17)	0.4046 (3)	0.30745 (16)	0.0507 (7)
O4	0.54793 (14)	0.2534 (3)	0.41891 (15)	0.0410 (6)
N1	0.60523 (12)	0.5385 (3)	0.53479 (14)	0.0155 (5)
H1	0.6243 (17)	0.470 (4)	0.5051 (19)	0.020 (8)*
N2	0.50238 (12)	0.3441 (3)	0.59248 (14)	0.0158 (5)
H2	0.4875 (16)	0.396 (4)	0.6259 (18)	0.013 (8)*
C1	0.61957 (14)	0.4670 (3)	0.61637 (16)	0.0176 (5)
H1A	0.6009	0.5431	0.6547	0.021*
C2	0.69850 (15)	0.4392 (4)	0.63986 (18)	0.0234 (6)
H2A	0.7230	0.5446	0.6414	0.028*
H2B	0.7185	0.3707	0.6002	0.028*
C3	0.71017 (15)	0.3558 (4)	0.72101 (18)	0.0240 (6)
H3A	0.7604	0.3339	0.7330	0.029*
H3B	0.6947	0.4291	0.7616	0.029*
C4	0.66895 (16)	0.1946 (4)	0.72184 (18)	0.0244 (6)
H4A	0.6752	0.1463	0.7745	0.029*
H4B	0.6877	0.1176	0.6848	0.029*
C5	0.58952 (15)	0.2218 (4)	0.69897 (17)	0.0207 (6)
H5A	0.5651	0.1163	0.6975	0.025*
H5B	0.5696	0.2903	0.7387	0.025*
C6	0.57805 (14)	0.3055 (3)	0.61764 (16)	0.0160 (5)
H6	0.5959	0.2312	0.5780	0.019*
C7	0.45702 (15)	0.1938 (3)	0.58195 (17)	0.0198 (6)
H7A	0.4616	0.1293	0.6305	0.024*
H7B	0.4737	0.1264	0.5398	0.024*
C8	0.37895 (15)	0.2367 (4)	0.56167 (17)	0.0219 (6)
H8A	0.3656	0.3212	0.5984	0.026*
H8B	0.3507	0.1393	0.5704	0.026*
C9	0.35957 (15)	0.2981 (4)	0.47688 (17)	0.0219 (6)

H9	0.3081	0.3170	0.4714	0.026*
C10	0.37587 (19)	0.1718 (4)	0.41449 (19)	0.0320 (7)
H10A	0.3628	0.2158	0.3625	0.048*
H10B	0.3493	0.0727	0.4220	0.048*
H10C	0.4258	0.1471	0.4195	0.048*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0130 (2)	0.0137 (2)	0.0158 (2)	−0.00162 (19)	−0.00138 (16)	0.00281 (19)
Cl1	0.0326 (4)	0.0214 (4)	0.0281 (4)	0.0029 (3)	0.0118 (3)	−0.0031 (3)
O1	0.0306 (14)	0.081 (2)	0.077 (2)	0.0053 (15)	0.0024 (14)	−0.0350 (19)
O2	0.0638 (18)	0.0272 (13)	0.0468 (16)	0.0020 (12)	0.0253 (13)	−0.0105 (11)
O3	0.083 (2)	0.0344 (15)	0.0368 (15)	0.0139 (14)	0.0160 (14)	0.0071 (12)
O4	0.0563 (16)	0.0321 (13)	0.0384 (14)	−0.0093 (12)	0.0264 (12)	−0.0074 (11)
N1	0.0175 (11)	0.0126 (11)	0.0162 (11)	−0.0016 (9)	−0.0004 (9)	0.0008 (9)
N2	0.0147 (11)	0.0144 (11)	0.0181 (12)	0.0006 (9)	0.0012 (9)	0.0003 (9)
C1	0.0196 (13)	0.0152 (14)	0.0176 (13)	−0.0007 (10)	−0.0002 (10)	0.0015 (10)
C2	0.0156 (13)	0.0272 (15)	0.0263 (15)	−0.0019 (12)	−0.0042 (11)	0.0046 (12)
C3	0.0200 (14)	0.0283 (16)	0.0224 (15)	0.0020 (12)	−0.0055 (11)	0.0033 (12)
C4	0.0244 (15)	0.0251 (15)	0.0224 (15)	0.0040 (12)	−0.0055 (12)	0.0040 (12)
C5	0.0219 (14)	0.0198 (14)	0.0200 (14)	−0.0008 (12)	−0.0009 (11)	0.0038 (11)
C6	0.0151 (12)	0.0150 (13)	0.0177 (13)	0.0022 (10)	−0.0002 (10)	0.0011 (10)
C7	0.0222 (14)	0.0135 (13)	0.0233 (14)	−0.0022 (11)	−0.0004 (11)	0.0030 (11)
C8	0.0198 (14)	0.0221 (15)	0.0234 (15)	−0.0068 (11)	−0.0014 (11)	0.0068 (12)
C9	0.0175 (13)	0.0216 (14)	0.0259 (15)	−0.0055 (11)	−0.0025 (11)	0.0056 (12)
C10	0.045 (2)	0.0202 (15)	0.0292 (17)	−0.0070 (14)	−0.0072 (14)	−0.0012 (13)

Geometric parameters (Å, °)

Cu1—N2	2.005 (2)	C3—H3A	0.9700
Cu1—N2^i	2.005 (2)	C3—H3B	0.9700
Cu1—N1	2.048 (2)	C4—C5	1.533 (4)
Cu1—N1^i	2.048 (2)	C4—H4A	0.9700
Cu1—O4	2.623 (2)	C4—H4B	0.9700
Cl1—O2	1.419 (2)	C5—C6	1.531 (4)
Cl1—O3	1.431 (3)	C5—H5A	0.9700
Cl1—O1	1.442 (3)	C5—H5B	0.9700
Cl1—O4	1.442 (2)	C6—H6	0.9800
N1—C1	1.499 (3)	C7—C8	1.525 (4)
N1—C9^i	1.500 (3)	C7—H7A	0.9700
N1—H1	0.85 (3)	C7—H7B	0.9700
N2—C6	1.489 (3)	C8—C9	1.531 (4)
N2—C7	1.490 (3)	C8—H8A	0.9700
N2—H2	0.77 (3)	C8—H8B	0.9700
C1—C6	1.525 (4)	C9—N1^i	1.500 (3)
C1—C2	1.526 (4)	C9—C10	1.517 (4)
C1—H1A	0.9800	C9—H9	0.9800

C2—C3	1.528 (4)	C10—H10A	0.9600
C2—H2A	0.9700	C10—H10B	0.9600
C2—H2B	0.9700	C10—H10C	0.9600
C3—C4	1.519 (4)		
N2—Cu1—N2^i	180.000 (1)	C2—C3—H3B	109.5
N2—Cu1—N1	85.04 (9)	H3A—C3—H3B	108.1
N2^i—Cu1—N1	94.96 (9)	C3—C4—C5	111.5 (2)
N2—Cu1—N1^i	94.96 (9)	C3—C4—H4A	109.3
N2^i—Cu1—N1^i	85.04 (9)	C5—C4—H4A	109.3
N1—Cu1—N1^i	180.00 (4)	C3—C4—H4B	109.3
N2—Cu1—O4	86.65 (9)	C5—C4—H4B	109.3
N2^i—Cu1—O4	93.35 (9)	H4A—C4—H4B	108.0
N1—Cu1—O4	84.11 (9)	C6—C5—C4	110.6 (2)
N1^i—Cu1—O4	95.89 (9)	C6—C5—H5A	109.5
O2—Cl1—O3	110.32 (16)	C4—C5—H5A	109.5
O2—Cl1—O1	110.74 (17)	C6—C5—H5B	109.5
O3—Cl1—O1	107.8 (2)	C4—C5—H5B	109.5
O2—Cl1—O4	111.10 (15)	H5A—C5—H5B	108.1
O3—Cl1—O4	108.71 (17)	N2—C6—C1	107.4 (2)
O1—Cl1—O4	108.06 (18)	N2—C6—C5	114.2 (2)
Cl1—O4—Cu1	122.78 (14)	C1—C6—C5	110.9 (2)
C1—N1—C9^i	114.4 (2)	N2—C6—H6	108.1
C1—N1—Cu1	107.59 (16)	C1—C6—H6	108.1
C9^i—N1—Cu1	121.75 (17)	C5—C6—H6	108.1
C1—N1—H1	104 (2)	N2—C7—C8	112.1 (2)
C9^i—N1—H1	107 (2)	N2—C7—H7A	109.2
Cu1—N1—H1	100 (2)	C8—C7—H7A	109.2
C6—N2—C7	113.0 (2)	N2—C7—H7B	109.2
C6—N2—Cu1	108.26 (16)	C8—C7—H7B	109.2
C7—N2—Cu1	116.42 (17)	H7A—C7—H7B	107.9
C6—N2—H2	108 (2)	C7—C8—C9	115.8 (2)
C7—N2—H2	107 (2)	C7—C8—H8A	108.3
Cu1—N2—H2	104 (2)	C9—C8—H8A	108.3
N1—C1—C6	106.9 (2)	C7—C8—H8B	108.3
N1—C1—C2	113.2 (2)	C9—C8—H8B	108.3
C6—C1—C2	111.2 (2)	H8A—C8—H8B	107.4
N1—C1—H1A	108.5	N1^i—C9—C10	112.6 (2)
C6—C1—H1A	108.5	N1^i—C9—C8	109.5 (2)
C2—C1—H1A	108.5	C10—C9—C8	112.6 (3)
C1—C2—C3	111.3 (2)	N1^i—C9—H9	107.2
C1—C2—H2A	109.4	C10—C9—H9	107.2
C3—C2—H2A	109.4	C8—C9—H9	107.2
C1—C2—H2B	109.4	C9—C10—H10A	109.5
C3—C2—H2B	109.4	C9—C10—H10B	109.5
H2A—C2—H2B	108.0	H10A—C10—H10B	109.5
C4—C3—C2	110.6 (2)	C9—C10—H10C	109.5

C4—C3—H3A	109.5	H10A—C10—H10C	109.5
C2—C3—H3A	109.5	H10B—C10—H10C	109.5
C4—C3—H3B	109.5		
O2—Cl1—O4—Cu1	−171.89 (17)	Cu1—N1—C1—C2	162.54 (19)
O3—Cl1—O4—Cu1	−50.3 (2)	N1—C1—C2—C3	−176.2 (2)
O1—Cl1—O4—Cu1	66.4 (2)	C6—C1—C2—C3	−55.9 (3)
N2—Cu1—O4—Cl1	−142.5 (2)	C1—C2—C3—C4	55.9 (3)
N2ⁱ—Cu1—O4—Cl1	37.5 (2)	C2—C3—C4—C5	−56.3 (3)
N1—Cu1—O4—Cl1	−57.18 (19)	C3—C4—C5—C6	56.4 (3)
N1ⁱ—Cu1—O4—Cl1	122.82 (19)	C7—N2—C6—C1	173.3 (2)
N2—Cu1—N1—C1	−13.38 (17)	Cu1—N2—C6—C1	42.8 (2)
N2ⁱ—Cu1—N1—C1	166.62 (17)	C7—N2—C6—C5	−63.3 (3)
O4—Cu1—N1—C1	−100.52 (17)	Cu1—N2—C6—C5	166.21 (19)
N2—Cu1—N1—C9ⁱ	−148.3 (2)	N1—C1—C6—N2	−54.8 (3)
N2ⁱ—Cu1—N1—C9ⁱ	31.7 (2)	C2—C1—C6—N2	−178.9 (2)
O4—Cu1—N1—C9ⁱ	124.6 (2)	N1—C1—C6—C5	179.8 (2)
N1—Cu1—N2—C6	−16.45 (17)	C2—C1—C6—C5	55.7 (3)
N1ⁱ—Cu1—N2—C6	163.55 (17)	C4—C5—C6—N2	−177.1 (2)
O4—Cu1—N2—C6	67.92 (18)	C4—C5—C6—C1	−55.7 (3)
N1—Cu1—N2—C7	−145.1 (2)	C6—N2—C7—C8	176.1 (2)
N1ⁱ—Cu1—N2—C7	34.9 (2)	Cu1—N2—C7—C8	−57.6 (3)
O4—Cu1—N2—C7	−60.68 (19)	N2—C7—C8—C9	74.2 (3)
C9ⁱ—N1—C1—C6	178.3 (2)	C7—C8—C9—N1ⁱ	−65.9 (3)
Cu1—N1—C1—C6	39.7 (2)	C7—C8—C9—C10	60.2 (3)
C9ⁱ—N1—C1—C2	−58.9 (3)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1	0.85 (3)	2.28 (3)	3.110 (4)	166 (2)
N2—H2···O3ⁱ	0.77 (3)	2.34 (3)	3.084 (4)	162 (3)

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

Fig. 1