Di-μ-chloro-bis{[N,N-bis(2-pyridylmethyl)-glycine-k⁴N,N',N'',O]copper(II)] diperchlorate acetonitrile tetrasolvate

Nielsen, Anne; McKenzie, Christine Joy; Bond, Andrew

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Anne Nielsen, Christine J. McKenzie and Andrew D. Bond*

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The title compound, $[Cu_2Cl_2(C_{14}H_{15}N_3O_2)_2](ClO_4)_2{\cdot}4C_2H_3N$, contains dichloro-bridged dicopper(II) complexes lying on centres of inversion. The crystal examined was twinned by a 180° rotation about c^*.

Comment

Reaction of bis(2-pyridylmethyl)glycine (bpgH) and $CuCl_2{\cdot}2H_2O$ in acidic methanol results in immediate precipitation of the title compound, (I). Compound (I) contains dichloro-bridged dicopper(II) complexes (Fig. 1) lying on centres of inversion, with the carboxylate groups protonated. The coordination geometry around the Cu^{II} atom (Table 1) is approximately octahedral, but exhibits significant elongation of the Cu1—O1 and Cu1—Cl1^i bonds [symmetry code: (i) $1-x, 1-y, 1-z$] on account of the Jahn–Teller distortion associated with Cu^{II}. The protonated carboxyl groups form hydrogen bonds to perchlorate anions (Table 2).

(I)

Experimental

Bis(2-pyridylmethyl)glycine (0.1573 g, 0.611 mmol) and $CuCl_2{\cdot}2H_2O$ (0.1047 g, 0.614 mmol) were dissolved in methanol (5 ml) and $HClO_4$ (0.25 ml of a 70% aqueous solution) was added. A turquoise powder (yield 0.2662 g, 93%) precipitated immediately. Recrystallization from hot acetonitrile afforded crystals of (I).

Crystal data

$[Cu_2Cl_2(C_{14}H_{15}N_3O_2)_2](ClO_4)_2{\cdot}$ $4C_2H_3N$	$\gamma = 97.159\,(4)°$
$M_r = 1075.68$	$V = 1127.58\,(17)$ Å³
Triclinic, $P\bar{1}$	$Z = 1$
$a = 7.1238\,(6)$ Å	$D_x = 1.584$ Mg m⁻³
$b = 10.6609\,(10)$ Å	Mo $K\alpha$ radiation
$c = 14.9894\,(13)$ Å	$\mu = 1.25$ mm⁻¹
$\alpha = 92.919\,(4)°$	$T = 180\,(2)$ K
$\beta = 91.266\,(4)°$	Plate, turquoise
	$0.24 \times 0.20 \times 0.05$ mm

Data collection

Bruker–Nonius X8APEX-II CCD diffractometer	26597 measured reflections
thin–slice ω and φ scans	8342 independent reflections
Absorption correction: multi-scan (*TWINABS*; Sheldrick, 2004)	4142 reflections with $I > 2\sigma(I)$
$T_{min} = 0.768$, $T_{max} = 0.940$	$R_{int} = 0.076$
	$\theta_{max} = 26.6°$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.073$	$w = 1/[\sigma^2(F_o^2) + (0.0828P)^2]$
$wR(F^2) = 0.191$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} < 0.001$
8342 reflections	$\Delta\rho_{max} = 1.11$ e Å^{-3}
289 parameters	$\Delta\rho_{min} = -0.65$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	1.970 (5)	Cu1—O1	2.316 (4)
Cu1—N2	2.076 (5)	Cu1—Cl1	2.2397 (17)
Cu1—N3	1.976 (5)	Cu1—Cl1^{i}	3.1116 (18)
N1—Cu1—N2	83.0 (2)	N3—Cu1—O1	91.58 (18)
N1—Cu1—N3	164.4 (2)	Cl1—Cu1—O1	100.18 (12)
N2—Cu1—N3	82.3 (2)	N1—Cu1—Cl1^{i}	84.87 (14)
N1—Cu1—Cl1	97.10 (15)	N2—Cu1—Cl1^{i}	84.60 (15)
N2—Cu1—Cl1	179.18 (17)	N3—Cu1—Cl1^{i}	88.40 (14)
N3—Cu1—Cl1	97.50 (15)	Cl1—Cu1—Cl1^{i}	94.61 (5)
N1—Cu1—O1	91.33 (17)	O1—Cu1—Cl1^{i}	165.08 (11)
N2—Cu1—O1	80.62 (18)		

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

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O2—H2⋯O2D^{ii}	0.84	1.88	2.720 (7)	176

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

The crystal was twinned by 180° rotation about c^*. The diffraction pattern was indexed using *CELL_NOW* (Bruker–Nonius, 2004) and integrated as a two-component twin using *SAINT-Plus* (Bruker, 2003). 8445 data (2549 unique; $R_{int} = 0.077$) were associated with component 1 only, 8423 data (2539 unique; $R_{int} = 0.084$) were associated with component 2 only, and 9729 data (3277 unique; $R_{int} = 0.076$) were overlapped. Refinement was performed using the HKLF5 format in *SHELXTL* (Sheldrick, 2000). H atoms bound to C atoms were positioned geometrically and allowed to ride during subsequent refinement, with C—H = 0.95 Å for Csp^2 or 0.99 Å for the methylene groups, and with $U_{iso}(H) = 1.2U_{eq}(C)$. The methyl groups of the acetonitrile molecules were positioned geometrically, with C—H = 0.98 Å and $U_{iso}(H) = 1.5U_{eq}(C)$, and allowed to rotate about their local threefold axes. In the final cycles of refinement, rotation was not permitted to aid convergence. The H atom of the hydroxyl group was

Figure 1
The dichloro-bridged dicopper(II) cationic complex in (I), showing displacement ellipsoids at the 50% probability level for non-H atoms. H atoms are shown as spheres of arbitrary radius. [Symmetry code (i) $1 - x$, $1 - y, 1 - z$.]

placed in the plane of the carboxyl group, so as to form the best hydrogen bond (AFIX 83 in *SHELXTL*), with O—H = 0.84 Å and $U_{iso}(H) = 1.5U_{eq}(O)$. The largest peak in the difference density lies in the vicinity of the perchlorate anion.

Data collection: *APEX2* (Bruker–Nonius, 2004); cell refinement: *SAINT-Plus* (Bruker, 2003); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

References

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Sheldrick, G. M. (2000). *SHELXTL*. Version 6.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2004). *TWINABS*. Version 1.05. Bruker–Nonius BV, Delft, The Netherlands.

supporting information

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S1. Comment

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S2. Experimental

Bis(2-pyridylmethyl)glycine (0.1573 g, 0.611 mmol) and $CuCl_2·2H_2O$ (0.1047 g, 0.614 mmol) were dissolved in methanol (5 ml) and $HClO_4$ (0.25 ml of a 70% aqueous solution) was added. A turquoise powder (yield 0.2662 g, 93%) precipitated immediately. Recrystallization from hot acetonitrile afforded crystals of (I).

S3. Refinement

The crystal was twinned by 180° rotation about *c**. The diffraction pattern was indexed using *CELL_NOW* (Bruker–Nonius, 2004) and integrated as a two-component twin using *SAINT-Plus* (Bruker, 2003). 8445 data (2549 unique; R_{int} = 0.077) were associated with component 1 only, 8423 data (2539 unique; R_{int} = 0.084) were associated with component 2 only, and 9729 data (3277 unique; R_{int} = 0.076) were overlapped. Refinement was performed using the HKLF5 format in *SHELXTL* (Sheldrick, 2000). H atoms bound to C atoms were positioned geometrically and allowed to ride during subsequent refinement, with C—H = 0.95 Å for Csp^2 or 0.99 Å for the methylene groups, and with $U_{iso}(H) = 1.2U_{eq}(C)$. The methyl groups of the acetonitrile molecules were positioned geometrically, with C—H = 0.98 Å and $U_{iso}(H) = 1.5U_{eq}(C)$, and allowed to rotate about their local threefold axes. In the final cycles of refinement, rotation was not permitted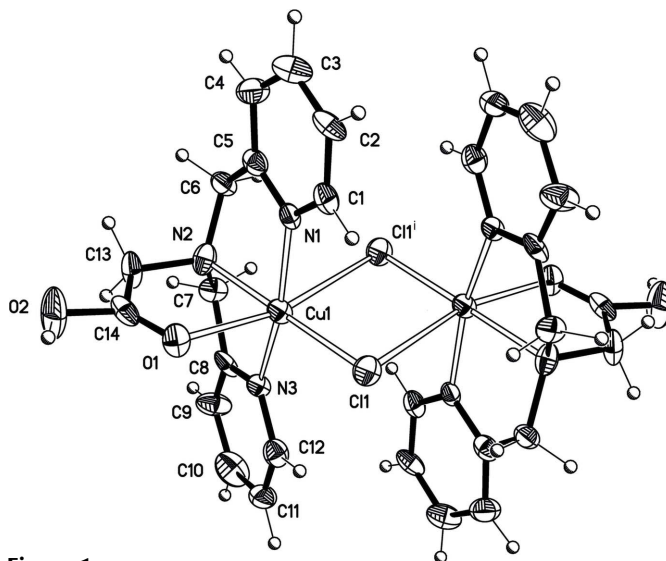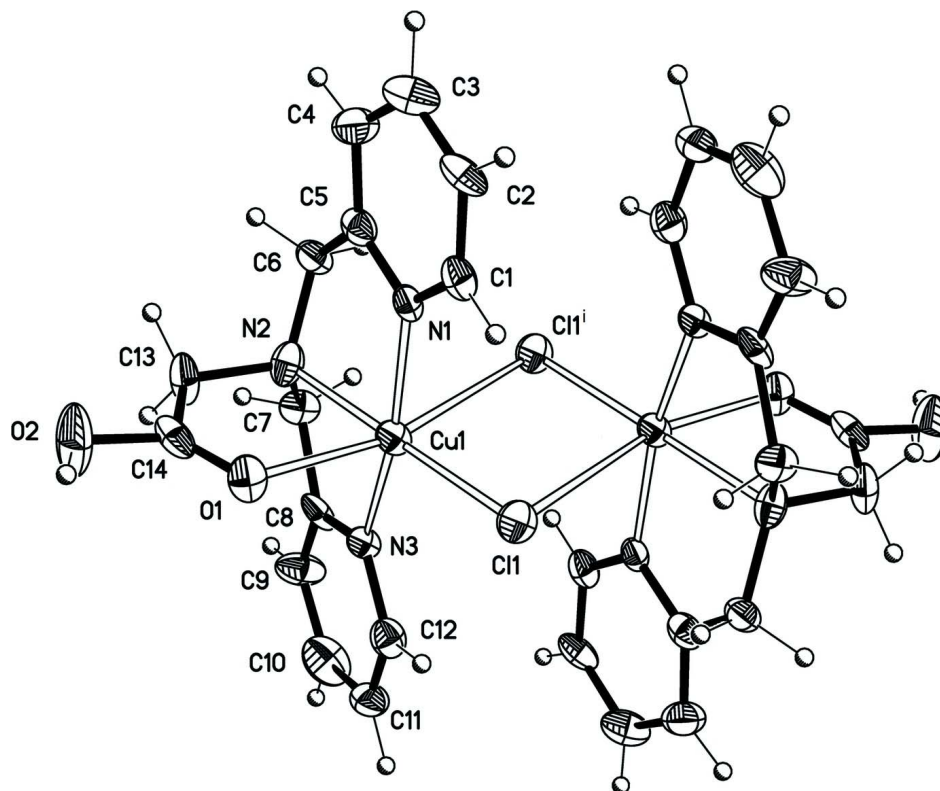 to aid convergence. The H atom of the hydroxyl group was placed in the plane of the carboxyl group, so as to form the best hydrogen bond (AFIX 83 in *SHELXTL*), with O—H = 0.84 Å and $U_{iso}(H) = 1.5U_{eq}(O)$. The largest peak in the difference density lies in the vicinity of the perchlorate anion.

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The dichloro-bridged dicopper(II) cationic complex in (I), showing displacement ellipsoids at the 50% probability level for non-H atoms. H atoms are shown as spheres of arbitrary radius.

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Crystal data

[Cu₂Cl₂(C₁₄H₁₅N₃O₂)₂](ClO₄)₂·4C₂H₃N
$M_r = 1075.68$
Triclinic, $P\bar{1}$
Hall symbol: -P 1
$a = 7.1238 (6)$ Å
$b = 10.6609 (10)$ Å
$c = 14.9894 (13)$ Å
$\alpha = 92.919 (4)°$
$\beta = 91.266 (4)°$
$\gamma = 97.159 (4)°$
$V = 1127.58 (17)$ Å³

$Z = 1$
$F(000) = 550$
$D_x = 1.584$ Mg m⁻³
Mo *Kα* radiation, $\lambda = 0.71073$ Å
Cell parameters from 2878 reflections
$\theta = 2.3–21.0°$
$\mu = 1.25$ mm⁻¹
$T = 180$ K
Plate, turquoise
$0.24 \times 0.20 \times 0.05$ mm

Data collection

Bruker–Nonius X8APEX-II CCD
  diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
thin–slice *ω* and *φ* scans

Absorption correction: multi-scan
  (TWINABS; Sheldrick, 2004)
$T_{min} = 0.768$, $T_{max} = 0.940$
26597 measured reflections
8342 independent reflections
4142 reflections with $I > 2\sigma(I)$

$R_{int} = 0.076$

$\theta_{max} = 26.6°$, $\theta_{min} = 3.5°$

$h = -8 \rightarrow 8$

$k = -13 \rightarrow 13$

$l = 0 \rightarrow 18$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.073$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.191$	
$S = 1.01$	H-atom parameters constrained
8342 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0828P)^2]$
289 parameters	where $P = (F_o^2 + 2F_c^2)/3$
0 restraints	$(\Delta/\sigma)_{max} < 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 1.11$ e Å^{-3}
	$\Delta\rho_{min} = -0.65$ 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.

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	0.42767 (10)	0.37182 (7)	0.41444 (5)	0.0218 (3)
Cl1	0.2439 (2)	0.41709 (15)	0.52801 (11)	0.0292 (5)
O1	0.2305 (5)	0.2095 (4)	0.3392 (3)	0.0290 (11)
O2	0.2394 (7)	0.0856 (5)	0.2135 (3)	0.0542 (15)
H2	0.1276	0.0586	0.2258	0.081*
N1	0.3488 (7)	0.4963 (4)	0.3332 (3)	0.0204 (12)
N2	0.6012 (7)	0.3314 (5)	0.3101 (4)	0.0289 (14)
N3	0.5673 (6)	0.2499 (4)	0.4749 (4)	0.0213 (12)
C1	0.1958 (8)	0.5590 (6)	0.3398 (4)	0.0253 (16)
H1A	0.1169	0.5453	0.3895	0.030*
C2	0.1491 (9)	0.6412 (6)	0.2783 (5)	0.0297 (17)
H2A	0.0410	0.6841	0.2861	0.036*
C3	0.2597 (10)	0.6612 (6)	0.2052 (5)	0.041 (2)
H3A	0.2319	0.7198	0.1625	0.050*
C4	0.4147 (10)	0.5932 (6)	0.1950 (5)	0.0352 (18)
H4A	0.4892	0.6008	0.1433	0.042*
C5	0.4578 (8)	0.5151 (6)	0.2609 (4)	0.0247 (16)
C6	0.6344 (8)	0.4497 (5)	0.2592 (4)	0.0251 (16)
H6A	0.6650	0.4278	0.1967	0.030*
H6B	0.7426	0.5069	0.2868	0.030*
C7	0.7790 (8)	0.3016 (6)	0.3560 (4)	0.0257 (16)
H7A	0.8602	0.3812	0.3747	0.031*

H7B	0.8504	0.2519	0.3142	0.031*
C8	0.7288 (8)	0.2269 (5)	0.4366 (4)	0.0250 (16)
C9	0.8453 (9)	0.1511 (6)	0.4729 (5)	0.0371 (19)
H9A	0.9591	0.1369	0.4444	0.044*
C10	0.7980 (10)	0.0943 (7)	0.5514 (5)	0.045 (2)
H10A	0.8813	0.0434	0.5784	0.054*
C11	0.6273 (9)	0.1121 (6)	0.5910 (5)	0.0322 (17)
H11A	0.5878	0.0711	0.6434	0.039*
C12	0.5204 (9)	0.1912 (6)	0.5506 (4)	0.0271 (17)
H12A	0.4051	0.2063	0.5774	0.033*
C13	0.5127 (8)	0.2235 (6)	0.2515 (5)	0.0312 (18)
H13A	0.5907	0.1531	0.2551	0.037*
H13B	0.5139	0.2494	0.1890	0.037*
C14	0.3092 (9)	0.1747 (6)	0.2742 (5)	0.0281 (17)
Cl2	0.2168 (2)	0.10340 (16)	0.78249 (12)	0.0333 (5)
O2A	0.4008 (6)	0.0842 (5)	0.8139 (4)	0.0628 (17)
O2B	0.1079 (8)	0.1460 (5)	0.8525 (4)	0.0686 (18)
O2C	0.2316 (8)	0.1957 (7)	0.7176 (4)	0.101 (3)
O2D	0.1254 (7)	−0.0110 (6)	0.7441 (5)	0.101 (3)
N1S	0.6069 (12)	0.2854 (7)	0.0246 (5)	0.080 (3)
C1S	0.6682 (11)	0.1934 (10)	0.0083 (5)	0.053 (2)
C2S	0.7474 (13)	0.0751 (8)	−0.0114 (6)	0.073 (3)
H2S1	0.8845	0.0878	0.0006	0.110*
H2S2	0.7217	0.0477	−0.0744	0.110*
H2S3	0.6881	0.0100	0.0266	0.110*
C4S	0.1761 (12)	0.3861 (8)	0.0051 (7)	0.076 (3)
H4S1	0.0797	0.4144	−0.0342	0.114*
H4S2	0.2226	0.3112	−0.0230	0.114*
H4S3	0.2816	0.4541	0.0150	0.114*
C3S	0.0933 (12)	0.3558 (8)	0.0901 (7)	0.053 (2)
N2S	0.0250 (13)	0.3353 (8)	0.1540 (6)	0.088 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0184 (4)	0.0197 (5)	0.0282 (5)	0.0045 (3)	0.0059 (4)	0.0023 (4)
Cl1	0.0257 (9)	0.0310 (11)	0.0326 (11)	0.0094 (8)	0.0101 (8)	0.0009 (9)
O1	0.019 (2)	0.031 (3)	0.036 (3)	−0.001 (2)	0.007 (2)	−0.006 (2)
O2	0.038 (3)	0.057 (4)	0.059 (4)	−0.011 (3)	0.001 (3)	−0.034 (3)
N1	0.021 (3)	0.015 (3)	0.025 (3)	0.000 (2)	0.004 (3)	−0.003 (2)
N2	0.026 (3)	0.035 (4)	0.027 (4)	0.010 (3)	0.004 (3)	−0.007 (3)
N3	0.020 (3)	0.018 (3)	0.029 (3)	0.008 (2)	0.013 (3)	0.003 (3)
C1	0.022 (4)	0.020 (4)	0.034 (4)	0.004 (3)	0.003 (3)	−0.004 (3)
C2	0.026 (4)	0.016 (4)	0.048 (5)	0.006 (3)	−0.003 (4)	0.006 (4)
C3	0.046 (5)	0.032 (5)	0.048 (5)	0.008 (4)	−0.001 (4)	0.017 (4)
C4	0.043 (5)	0.033 (5)	0.029 (5)	0.000 (4)	0.001 (4)	0.009 (4)
C5	0.025 (4)	0.019 (4)	0.028 (4)	−0.001 (3)	−0.008 (3)	0.000 (3)
C6	0.027 (4)	0.018 (4)	0.031 (4)	0.004 (3)	0.006 (3)	0.004 (3)

C7	0.017 (3)	0.030 (4)	0.032 (4)	0.007 (3)	0.009 (3)	0.007 (3)
C8	0.021 (4)	0.011 (4)	0.043 (5)	−0.001 (3)	0.007 (3)	−0.001 (3)
C9	0.030 (4)	0.036 (5)	0.049 (5)	0.008 (3)	0.017 (4)	0.019 (4)
C10	0.037 (5)	0.035 (5)	0.067 (6)	0.019 (4)	−0.003 (4)	0.005 (4)
C11	0.043 (4)	0.024 (4)	0.033 (5)	0.010 (3)	0.008 (4)	0.007 (4)
C12	0.024 (4)	0.025 (4)	0.033 (5)	0.004 (3)	0.003 (3)	−0.002 (3)
C13	0.024 (4)	0.028 (4)	0.039 (5)	−0.003 (3)	0.009 (3)	−0.017 (4)
C14	0.027 (4)	0.015 (4)	0.042 (5)	0.004 (3)	−0.011 (4)	0.001 (4)
Cl2	0.0282 (10)	0.0325 (11)	0.0394 (12)	0.0036 (8)	0.0058 (9)	0.0007 (10)
O2A	0.028 (3)	0.059 (4)	0.101 (5)	0.005 (3)	−0.021 (3)	0.013 (3)
O2B	0.076 (4)	0.075 (4)	0.058 (4)	0.022 (3)	0.033 (3)	−0.010 (3)
O2C	0.071 (4)	0.161 (7)	0.095 (5)	0.066 (4)	0.043 (4)	0.086 (5)
O2D	0.034 (3)	0.066 (5)	0.192 (8)	−0.008 (3)	0.001 (4)	−0.074 (5)
N1S	0.109 (7)	0.066 (6)	0.067 (6)	0.023 (5)	0.036 (5)	−0.006 (5)
C1S	0.043 (5)	0.083 (8)	0.024 (5)	−0.022 (5)	0.003 (4)	0.008 (5)
C2S	0.082 (7)	0.065 (7)	0.069 (7)	−0.001 (5)	0.022 (6)	−0.009 (5)
C4S	0.068 (6)	0.075 (7)	0.084 (8)	0.008 (5)	0.000 (6)	−0.016 (6)
C3S	0.045 (6)	0.051 (6)	0.060 (7)	0.010 (5)	−0.013 (5)	−0.016 (6)
N2S	0.112 (8)	0.079 (7)	0.073 (7)	0.005 (6)	0.006 (6)	0.007 (6)

Geometric parameters (Å, º)

Cu1—N1	1.970 (5)	C7—H7A	0.990
Cu1—N2	2.076 (5)	C7—H7B	0.990
Cu1—N3	1.976 (5)	C8—C9	1.353 (8)
Cu1—O1	2.316 (4)	C9—C10	1.380 (9)
Cu1—Cl1	2.2397 (17)	C9—H9A	0.950
Cu1—Cl1^i	3.1116 (18)	C10—C11	1.394 (8)
O1—C14	1.200 (7)	C10—H10A	0.950
O2—C14	1.323 (8)	C11—C12	1.360 (8)
O2—H2	0.840	C11—H11A	0.950
N1—C1	1.350 (7)	C12—H12A	0.950
N1—C5	1.355 (7)	C13—C14	1.530 (8)
N2—C13	1.478 (7)	C13—H13A	0.990
N2—C6	1.503 (7)	C13—H13B	0.990
N2—C7	1.504 (7)	Cl2—O2D	1.398 (5)
N3—C8	1.341 (7)	Cl2—O2B	1.408 (5)
N3—C12	1.351 (7)	Cl2—O2C	1.415 (6)
C1—C2	1.368 (8)	Cl2—O2A	1.425 (5)
C1—H1A	0.950	N1S—C1S	1.140 (10)
C2—C3	1.375 (9)	C1S—C2S	1.465 (12)
C2—H2A	0.950	C2S—H2S1	0.980
C3—C4	1.401 (9)	C2S—H2S2	0.980
C3—H3A	0.950	C2S—H2S3	0.980
C4—C5	1.377 (8)	C4S—C3S	1.451 (12)
C4—H4A	0.950	C4S—H4S1	0.980
C5—C6	1.513 (8)	C4S—H4S2	0.980
C6—H6A	0.990	C4S—H4S3	0.980

C6—H6B	0.990	C3S—N2S	1.103 (10)
C7—C8	1.506 (8)		
N1—Cu1—N2	83.0 (2)	N2—C7—C8	109.7 (5)
N1—Cu1—N3	164.4 (2)	N2—C7—H7A	109.7
N2—Cu1—N3	82.3 (2)	C8—C7—H7A	109.7
N1—Cu1—Cl1	97.10 (15)	N2—C7—H7B	109.7
N2—Cu1—Cl1	179.18 (17)	C8—C7—H7B	109.7
N3—Cu1—Cl1	97.50 (15)	H7A—C7—H7B	108.2
N1—Cu1—O1	91.33 (17)	N3—C8—C9	122.0 (6)
N2—Cu1—O1	80.62 (18)	N3—C8—C7	114.9 (5)
N3—Cu1—O1	91.58 (18)	C9—C8—C7	122.8 (6)
Cl1—Cu1—O1	100.18 (12)	C8—C9—C10	119.7 (6)
N1—Cu1—Cl1ⁱ	84.87 (14)	C8—C9—H9A	120.1
N2—Cu1—Cl1ⁱ	84.60 (15)	C10—C9—H9A	120.1
N3—Cu1—Cl1ⁱ	88.40 (14)	C9—C10—C11	119.6 (6)
Cl1—Cu1—Cl1ⁱ	94.61 (5)	C9—C10—H10A	120.2
O1—Cu1—Cl1ⁱ	165.08 (11)	C11—C10—H10A	120.2
C14—O1—Cu1	108.6 (4)	C12—C11—C10	116.5 (6)
C14—O2—H2	109.5	C12—C11—H11A	121.7
C1—N1—C5	117.6 (5)	C10—C11—H11A	121.7
C1—N1—Cu1	127.3 (4)	N3—C12—C11	124.4 (6)
C5—N1—Cu1	115.0 (4)	N3—C12—H12A	117.8
C13—N2—C6	110.8 (5)	C11—C12—H12A	117.8
C13—N2—C7	111.6 (5)	N2—C13—C14	114.5 (5)
C6—N2—C7	112.2 (5)	N2—C13—H13A	108.6
C13—N2—Cu1	111.5 (4)	C14—C13—H13A	108.6
C6—N2—Cu1	106.2 (3)	N2—C13—H13B	108.6
C7—N2—Cu1	104.1 (4)	C14—C13—H13B	108.6
C8—N3—C12	117.6 (5)	H13A—C13—H13B	107.6
C8—N3—Cu1	115.0 (4)	O1—C14—O2	126.3 (6)
C12—N3—Cu1	127.3 (4)	O1—C14—C13	124.4 (6)
N1—C1—C2	123.1 (6)	O2—C14—C13	109.3 (6)
N1—C1—H1A	118.4	O2D—Cl2—O2B	109.2 (4)
C2—C1—H1A	118.4	O2D—Cl2—O2C	109.4 (5)
C1—C2—C3	119.5 (6)	O2B—Cl2—O2C	108.0 (4)
C1—C2—H2A	120.3	O2D—Cl2—O2A	108.9 (3)
C3—C2—H2A	120.3	O2B—Cl2—O2A	111.4 (4)
C2—C3—C4	118.3 (7)	O2C—Cl2—O2A	109.9 (3)
C2—C3—H3A	120.8	N1S—C1S—C2S	179.3 (10)
C4—C3—H3A	120.8	C1S—C2S—H2S1	109.8
C5—C4—C3	119.2 (6)	C1S—C2S—H2S2	109.6
C5—C4—H4A	120.4	H2S1—C2S—H2S2	109.5
C3—C4—H4A	120.4	C1S—C2S—H2S3	109.0
N1—C5—C4	122.1 (6)	H2S1—C2S—H2S3	109.5
N1—C5—C6	115.8 (5)	H2S2—C2S—H2S3	109.5
C4—C5—C6	122.0 (6)	C3S—C4S—H4S1	109.1
N2—C6—C5	109.1 (5)	C3S—C4S—H4S2	110.1

N2—C6—H6A	109.9	H4S1—C4S—H4S2	109.5
C5—C6—H6A	109.9	C3S—C4S—H4S3	109.2
N2—C6—H6B	109.9	H4S1—C4S—H4S3	109.4
C5—C6—H6B	109.9	H4S2—C4S—H4S3	109.5
H6A—C6—H6B	108.3	N2S—C3S—C4S	177.3 (11)
N1—Cu1—O1—C14	81.7 (4)	Cu1—N1—C1—C2	−177.9 (5)
N3—Cu1—O1—C14	−82.9 (4)	N1—C1—C2—C3	0.9 (10)
N2—Cu1—O1—C14	−1.0 (4)	C1—C2—C3—C4	1.8 (10)
Cl1—Cu1—O1—C14	179.2 (4)	C2—C3—C4—C5	−4.0 (10)
Cl1ⁱ—Cu1—O1—C14	6.8 (7)	C1—N1—C5—C4	−1.1 (8)
N3—Cu1—N1—C1	−174.2 (7)	Cu1—N1—C5—C4	175.9 (5)
N2—Cu1—N1—C1	165.5 (5)	C1—N1—C5—C6	176.3 (5)
Cl1—Cu1—N1—C1	−15.3 (5)	Cu1—N1—C5—C6	−6.7 (6)
O1—Cu1—N1—C1	85.1 (5)	C3—C4—C5—N1	3.8 (10)
Cl1ⁱ—Cu1—N1—C1	−109.4 (5)	C3—C4—C5—C6	−173.4 (6)
N3—Cu1—N1—C5	9.1 (10)	C13—N2—C6—C5	86.8 (6)
N2—Cu1—N1—C5	−11.2 (4)	C7—N2—C6—C5	−147.6 (5)
Cl1—Cu1—N1—C5	168.0 (4)	Cu1—N2—C6—C5	−34.5 (6)
O1—Cu1—N1—C5	−91.6 (4)	N1—C5—C6—N2	28.6 (7)
Cl1ⁱ—Cu1—N1—C5	73.9 (4)	C4—C5—C6—N2	−154.0 (6)
N1—Cu1—N2—C13	−95.3 (4)	C13—N2—C7—C8	−81.5 (6)
N3—Cu1—N2—C13	90.1 (4)	C6—N2—C7—C8	153.3 (5)
O1—Cu1—N2—C13	−2.8 (4)	Cu1—N2—C7—C8	38.9 (6)
Cl1ⁱ—Cu1—N2—C13	179.2 (4)	C12—N3—C8—C9	−2.0 (9)
N1—Cu1—N2—C6	25.6 (4)	Cu1—N3—C8—C9	176.3 (5)
N3—Cu1—N2—C6	−149.0 (4)	C12—N3—C8—C7	−176.2 (5)
O1—Cu1—N2—C6	118.1 (4)	Cu1—N3—C8—C7	2.1 (7)
Cl1ⁱ—Cu1—N2—C6	−59.9 (4)	N2—C7—C8—N3	−28.9 (7)
N1—Cu1—N2—C7	144.2 (4)	N2—C7—C8—C9	156.8 (6)
N3—Cu1—N2—C7	−30.4 (4)	N3—C8—C9—C10	0.4 (10)
O1—Cu1—N2—C7	−123.3 (4)	C7—C8—C9—C10	174.2 (6)
Cl1ⁱ—Cu1—N2—C7	58.7 (3)	C8—C9—C10—C11	2.3 (11)
N1—Cu1—N3—C8	−3.4 (10)	C9—C10—C11—C12	−3.1 (10)
N2—Cu1—N3—C8	17.0 (4)	C8—N3—C12—C11	1.0 (9)
Cl1—Cu1—N3—C8	−162.2 (4)	Cu1—N3—C12—C11	−177.1 (5)
O1—Cu1—N3—C8	97.3 (4)	C10—C11—C12—N3	1.5 (10)
Cl1ⁱ—Cu1—N3—C8	−67.8 (4)	C6—N2—C13—C14	−112.4 (6)
N1—Cu1—N3—C12	174.7 (6)	C7—N2—C13—C14	121.7 (5)
N2—Cu1—N3—C12	−164.9 (5)	Cu1—N2—C13—C14	5.8 (7)
Cl1—Cu1—N3—C12	15.9 (5)	Cu1—O1—C14—O2	−178.2 (5)
O1—Cu1—N3—C12	−84.6 (5)	Cu1—O1—C14—C13	4.9 (7)
Cl1ⁱ—Cu1—N3—C12	110.3 (5)	N2—C13—C14—O1	−7.7 (9)
C5—N1—C1—C2	−1.3 (9)	N2—C13—C14—O2	175.0 (6)

Symmetry code: (i) −x+1, −y+1, −z+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O2*D*[ii]	0.84	1.88	2.720 (7)	176

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