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(Acetonitrile)[bis(2-pyridylmethyl)-amine]bis(perchlorato)copper(II)

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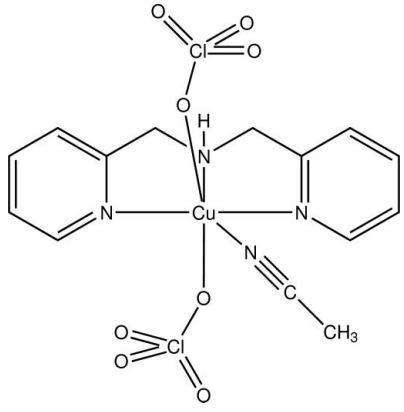
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.011 Å; disorder in main residue; R factor = 0.064; wR factor = 0.193; data-to-parameter ratio = 13.6.

In the title compound, $[Cu(ClO_4)_2(C_{12}H_{13}N_3)(C_2H_3N)]$, the Cu^{II} atom is six-coordinate in a Jahn–Teller distorted octahedral geometry, with coordination by the tridentate chelating ligand, an acetonitrile molecule, and two axial perchlorate anions. The tridentate ligand bis(2-pyridylmethyl)amine chelates meridionally and equatorially while an acetonitrile molecule is coordinated at the fourth equatorial site. The two perchlorate anions are disordered with site occupancy factors of 0.72/0.28. The amine H is involved in intramolecular hydrogen bonding to the perchlorate O atoms and there are extensive but weak intermolecular C—H···O interactions.

Related literature

For related literature, see: Belle *et al.* (2002); Gultneh *et al.* (1999); Humphreys *et al.* (2002); Palaniandavar *et al.* (1995).



Experimental

Crystal data

$[Cu(ClO_4)_2(C_{12}H_{13}N_3)(C_2H_3N)]$
M_r = 502.75
Monoclinic, $P2_1/c$
a = 8.3046 (16) Å
b = 31.453 (4) Å
c = 8.4978 (11) Å
β = 118.646 (10)°
V = 1948.0 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.45 mm^{-1}
T = 293 (2) K
0.45 × 0.21 × 0.07 mm

Data collection

Bruker P4S diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.757, T_{max} = 0.964
(expected range = 0.709–0.904)
4638 measured reflections
4347 independent reflections
2718 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
3 standard reflections
every 97 reflections
intensity decay: <2%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.193
S = 1.04
4347 reflections
320 parameters
92 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N—H0A···O22A	0.91	2.45	2.89 (3)	110
N—H0A···O23	0.91	2.30	3.084 (12)	144
N—H0A···O23^{i}	0.91	2.50	3.317 (10)	150
C2—H21···O13A^{ii}	0.96	2.23	2.98 (2)	133
C2—H22···O14^{iii}	0.96	2.36	3.103 (14)	134
C1A—H1AA···O12^{ii}	0.93	2.46	3.176 (9)	134
C3A—H3AA···O23^{iv}	0.93	2.53	3.376 (15)	152
C3A—H3AA···O23A^{iv}	0.93	2.29	2.993 (14)	133
C6A—H6AA···O21^{i}	0.97	2.56	3.381 (9)	143
C2B—H2BA···O14A^{v}	0.93	2.35	3.112 (16)	140
C3B—H3BA···O11^{vi}	0.93	2.56	3.429 (10)	156
C4B—H4BA···O24A^{vii}	0.93	2.25	3.06 (3)	145
C6B—H6BA···O12	0.97	2.56	3.425 (13)	149
C6B—H6BB···O24A^{vii}	0.97	2.51	3.211 (16)	129

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

Data collection: *XSCANS* (Bruker, 1997); cell refinement: *XSCANS*; data reduction: *XSCANS*; 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2058).

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supporting information

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(Acetonitrile)[bis(2-pyridylmethyl)amine]bis(perchlorato)copper(II)

Ray J. Butcher, Yohannes T. Tesema, Teshome B. Yisgedu and Yilma Gultneh

S1. Comment

Bis(2-pyridylmethyl)amine (L^1) has been used as a chelating ligand for several metal ions, as a single unit, or as two or more units bridged by other groups (such as *m*-xylyl spaces or aliphatic hydrocarbon chains) through the amine N atom (Gultneh *et al.*, 1999; Palaniandavar *et al.*, 1995; Belle *et al.*, 2002; Humphreys *et al.*, 2002). We report here the structure of the copper (II) complex of the ligand L^1. The complex was synthesized by the reaction of L^1 with $Cu(ClO_4)_2.6H_2O$ in acetonitrile.

The crystal structure shows that Cu^{II} is six-coordinate in a Jahn-Teller distorted geometry with coordination by the tridentate chelating ligand, an acetonitrile molecule, and two axial perchlorate anions (Fig. 1.). The tridentate ligand L^1 is chelating meridionally and equatorially while an acetonitrile molecule is coordinated at the fourth equatorial site. One axial perchlorate group is at a Cu^{II}—$OClO_3^-$ distance of 2.455 (9) Å while the other is at 2.828 (5) Å consistent with its expected Jahn-Teller elongation (O—Cu—O angle 169.1 (2)°). The mutually *trans* Cu—N_{py} distances are 1.980 (5) Å and 1.984 (5) Å and span an angle of 165.3 (2)°. The Cu—N_{amine} bond distance is 1.991 (5) Å. The Cu—$N_{acetonitrile}$ bond distance of 1.980 (5) Å is comparable to the Cu—N distances of the N atoms. The amine H is involved in intramolecular hydrogen bonding to the perchlorate O atoms and there are extensive but weak intermolecular C—H···O interactions. (Table 1.).

S2. Experimental

The title compound, bis(2-pyridylmethyl)amine copper(II) acetonitrile bis(perchlorate), was obtained by refluxing bis(2-pyridylmethyl)amine (2 mmol) and copper(II) perchlorate hexahydrate (2 mmol) in 200 ml of acetonitrile for 1 h. The product deposited on cooling the solution. Suitable crystals suited for crystallographic structure determination were obtained by slow diffusion of diethyl ether into the nitromethane solution of the complex.

S3. Refinement

The two perchlorate anions are disordered such that O11 and O21 are unique and the remaining O atoms are disordered over two conformations with occupancy factors of 0.708 (9), 0.292 (9) and 0.73 (3), 0.27 (3), respectively. The H atoms were idealized with an N—H distance of 0.91 and C—H distances were idealized at 0.93 (aromatic C—H), 0.96 (CH_3), and 0.97 (CH_2) Å and $U_{iso}(H) = 1.2U_{eq}(C)$ ($1.5U_{eq}(C)$ for the CH_3 protons).

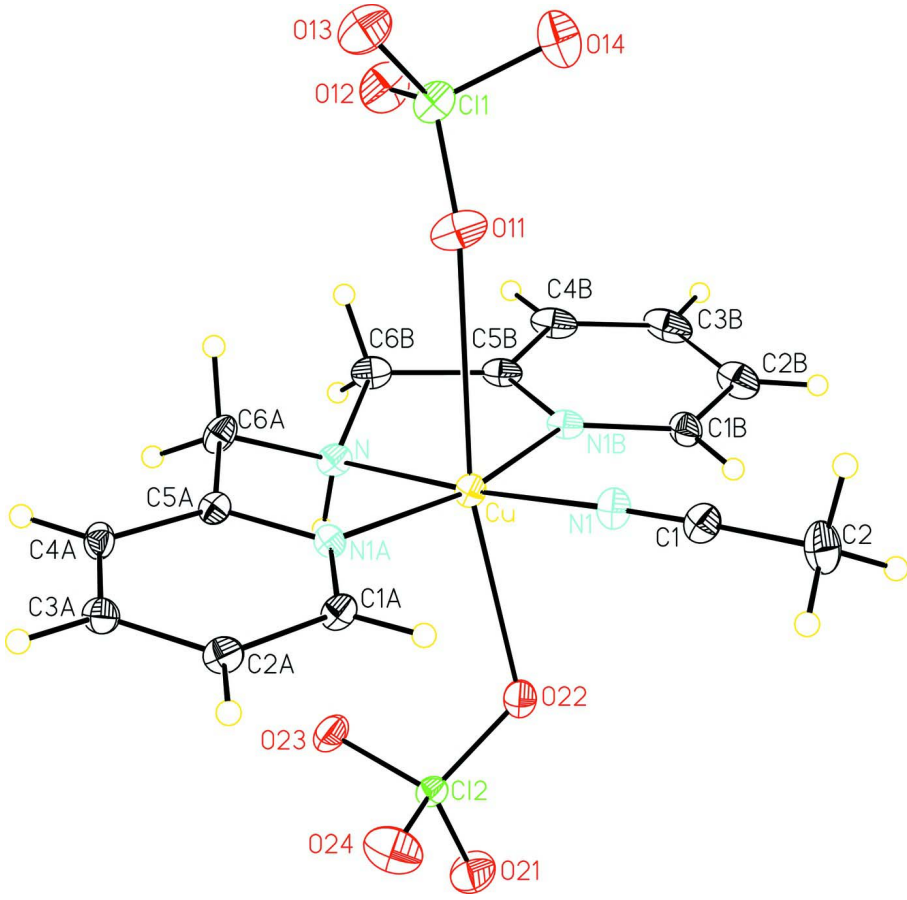

Figure 1

The title compound with numbering scheme used. Ellipsoids are drawn at the 20% probability level.

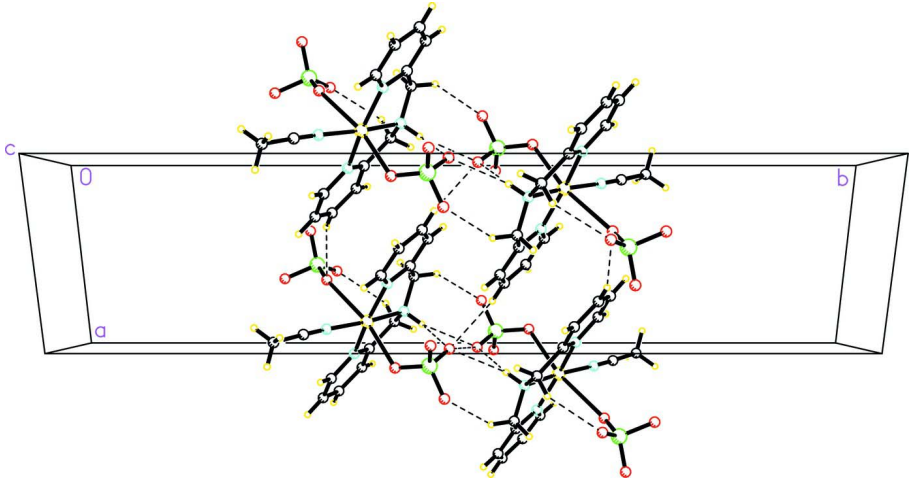

Figure 2

The packing arrangement viewed down the *c* axis showing the intramolecular N—H···O and intermolecular C—H···O interactions in dashed lines.

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Crystal data

$[Cu(ClO_4)_2(C_{12}H_{13}N_3)(C_2H_3N)]$
$M_r = 502.75$
Monoclinic, $P2_1/c$
Hall symbol: -P2ybc
$a = 8.3046$ (16) Å
$b = 31.453$ (4) Å
$c = 8.4978$ (11) Å
$\beta = 118.646$ (10)°
$V = 1948.0$ (5) Å^3
$Z = 4$
$F(000) = 1020$
$D_x = 1.714$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 54 reflections
$\theta = 2.6$–13.1°
$\mu = 1.45$ mm^{-1}
$T = 293$ K
Plate, blue
0.45 × 0.21 × 0.07 mm

Data collection

Bruker P4S diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$2\theta/\omega$ scans
Absorption correction: empirical (using intensity measurements) via psi scans (North *et al.*, 1968)
$T_{min} = 0.757$, $T_{max} = 0.964$
4638 measured reflections
4347 independent reflections
2718 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.6°$
$h = 0 \rightarrow 9$
$k = -40 \rightarrow 0$
$l = -11 \rightarrow 9$
3 standard reflections every 97 reflections
intensity decay: <2

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.064$
$wR(F^2) = 0.193$
$S = 1.04$
4347 reflections
320 parameters
92 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0863P)^2 + 3.5739P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.46$ 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}	Occ. (<1)
Cu	0.85396 (9)	0.12165 (2)	−0.01007 (9)	0.0455 (2)	
Cl1	0.5466 (2)	0.19134 (7)	−0.4772 (2)	0.0704 (5)	
Cl2	1.07924 (18)	0.04196 (5)	0.29953 (18)	0.0480 (4)	

O11	0.6293 (8)	0.1760 (2)	−0.2975 (7)	0.104 (2)	
O12	0.5827 (15)	0.1680 (3)	−0.5954 (12)	0.107 (4)	0.708 (9)
O13	0.3563 (10)	0.1998 (4)	−0.5489 (12)	0.106 (3)	0.708 (9)
O14	0.6252 (16)	0.2343 (3)	−0.4642 (15)	0.128 (4)	0.708 (9)
O12A	0.412 (3)	0.1546 (6)	−0.561 (3)	0.123 (7)	0.292 (9)
O13A	0.673 (3)	0.1865 (9)	−0.538 (3)	0.121 (8)	0.292 (9)
O14A	0.449 (3)	0.2264 (6)	−0.510 (3)	0.134 (8)	0.292 (9)
O21	1.2524 (7)	0.0234 (2)	0.4056 (8)	0.105 (2)	
O22	1.0940 (12)	0.0848 (3)	0.2525 (18)	0.073 (3)	0.73 (3)
O23	0.9968 (17)	0.0176 (3)	0.1363 (12)	0.091 (4)	0.73 (3)
O24	0.9656 (18)	0.0399 (5)	0.378 (2)	0.114 (5)	0.73 (3)
O22A	1.083 (3)	0.0726 (9)	0.180 (4)	0.061 (5)	0.27 (3)
O23A	0.945 (3)	0.0114 (7)	0.200 (4)	0.103 (11)	0.27 (3)
O24A	1.031 (4)	0.0626 (11)	0.422 (3)	0.120 (13)	0.27 (3)
N	0.8033 (7)	0.07655 (17)	−0.1923 (6)	0.0535 (12)	
H0A	0.8722	0.0536	−0.1326	0.064*	
N1	0.8876 (7)	0.16941 (18)	0.1547 (7)	0.0578 (13)	
N1A	0.6448 (6)	0.09486 (15)	0.0037 (6)	0.0437 (10)	
N1B	1.0370 (7)	0.14026 (16)	−0.0821 (7)	0.0505 (12)	
C1	0.9117 (9)	0.1962 (2)	0.2536 (9)	0.0592 (16)	
C2	0.9472 (12)	0.2296 (3)	0.3847 (12)	0.085 (2)	
H21	0.9179	0.2194	0.4746	0.127*	
H22	0.8726	0.2539	0.3259	0.127*	
H23	1.0744	0.2375	0.4402	0.127*	
C1A	0.5988 (8)	0.1008 (2)	0.1336 (7)	0.0501 (14)	
H1AA	0.6635	0.1206	0.2237	0.060*	
C2A	0.4574 (8)	0.0783 (2)	0.1363 (8)	0.0568 (16)	
H2AA	0.4302	0.0820	0.2296	0.068*	
C3A	0.3585 (8)	0.0508 (2)	0.0004 (9)	0.0579 (16)	
H3AA	0.2603	0.0361	−0.0017	0.069*	
C4A	0.4043 (8)	0.04453 (19)	−0.1353 (9)	0.0544 (15)	
H4AA	0.3383	0.0256	−0.2285	0.065*	
C5A	0.5498 (7)	0.06705 (18)	−0.1285 (7)	0.0440 (12)	
C6A	0.6090 (8)	0.0636 (2)	−0.2696 (8)	0.0608 (17)	
H6AA	0.5946	0.0345	−0.3126	0.073*	
H6AB	0.5331	0.0818	−0.3704	0.073*	
C1B	1.1723 (8)	0.1693 (2)	0.0060 (9)	0.0613 (17)	
H1BA	1.1857	0.1809	0.1123	0.074*	
C2B	1.2893 (10)	0.1821 (3)	−0.0557 (13)	0.081 (2)	
H2BA	1.3817	0.2018	0.0070	0.097*	
C3B	1.2643 (11)	0.1644 (3)	−0.2174 (13)	0.090 (3)	
H3BA	1.3384	0.1731	−0.2658	0.108*	
C4B	1.1319 (11)	0.1345 (3)	−0.3037 (11)	0.075 (2)	
H4BA	1.1176	0.1220	−0.4087	0.090*	
C5B	1.0171 (9)	0.1229 (2)	−0.2317 (9)	0.0580 (16)	
C6B	0.8664 (10)	0.0902 (2)	−0.3200 (8)	0.0624 (17)	
H6BA	0.7647	0.1024	−0.4259	0.075*	
H6BB	0.9120	0.0659	−0.3569	0.075*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu	0.0421 (4)	0.0597 (5)	0.0456 (4)	−0.0037 (3)	0.0299 (3)	−0.0057 (3)
Cl1	0.0599 (10)	0.0979 (14)	0.0629 (10)	0.0036 (9)	0.0371 (9)	−0.0078 (9)
Cl2	0.0430 (7)	0.0613 (9)	0.0422 (7)	−0.0001 (6)	0.0225 (6)	−0.0009 (6)
O11	0.086 (4)	0.151 (6)	0.072 (4)	0.032 (4)	0.036 (3)	0.023 (4)
O12	0.120 (8)	0.114 (8)	0.098 (6)	0.021 (6)	0.061 (6)	−0.035 (5)
O13	0.070 (5)	0.147 (9)	0.101 (6)	0.021 (5)	0.041 (5)	0.001 (6)
O14	0.146 (9)	0.093 (7)	0.154 (9)	−0.027 (6)	0.079 (8)	−0.022 (6)
O12A	0.110 (12)	0.124 (13)	0.105 (11)	−0.020 (11)	0.026 (10)	−0.011 (11)
O13A	0.122 (16)	0.131 (18)	0.163 (16)	0.012 (13)	0.110 (13)	0.011 (14)
O14A	0.122 (13)	0.092 (12)	0.166 (13)	0.027 (12)	0.050 (13)	0.006 (12)
O21	0.066 (3)	0.113 (5)	0.103 (5)	0.021 (3)	0.014 (3)	0.016 (4)
O22	0.070 (4)	0.064 (5)	0.072 (6)	−0.010 (4)	0.023 (4)	−0.004 (4)
O23	0.099 (7)	0.075 (6)	0.057 (5)	−0.009 (5)	0.003 (5)	−0.010 (4)
O24	0.127 (9)	0.137 (11)	0.137 (10)	0.022 (8)	0.111 (9)	0.025 (8)
O22A	0.065 (7)	0.066 (9)	0.065 (9)	0.014 (7)	0.041 (8)	0.020 (7)
O23A	0.101 (19)	0.106 (19)	0.08 (2)	−0.064 (15)	0.026 (15)	−0.010 (14)
O24A	0.22 (4)	0.11 (2)	0.076 (16)	−0.01 (2)	0.11 (2)	−0.034 (16)
N	0.057 (3)	0.071 (3)	0.045 (3)	0.001 (2)	0.035 (2)	−0.003 (2)
N1	0.056 (3)	0.065 (3)	0.065 (3)	−0.009 (3)	0.039 (3)	−0.014 (3)
N1A	0.040 (2)	0.049 (3)	0.050 (3)	0.000 (2)	0.028 (2)	0.000 (2)
N1B	0.049 (3)	0.061 (3)	0.054 (3)	0.013 (2)	0.035 (2)	0.014 (2)
C1	0.049 (3)	0.074 (5)	0.060 (4)	−0.004 (3)	0.030 (3)	−0.005 (3)
C2	0.094 (6)	0.067 (5)	0.100 (6)	−0.017 (4)	0.053 (5)	−0.029 (4)
C1A	0.042 (3)	0.074 (4)	0.042 (3)	−0.002 (3)	0.026 (3)	−0.006 (3)
C2A	0.043 (3)	0.084 (5)	0.054 (4)	0.001 (3)	0.032 (3)	0.007 (3)
C3A	0.039 (3)	0.072 (4)	0.066 (4)	0.001 (3)	0.028 (3)	0.015 (3)
C4A	0.038 (3)	0.049 (3)	0.066 (4)	−0.002 (3)	0.017 (3)	−0.002 (3)
C5A	0.036 (3)	0.048 (3)	0.048 (3)	0.008 (2)	0.020 (2)	−0.002 (2)
C6A	0.049 (3)	0.084 (5)	0.048 (3)	−0.004 (3)	0.023 (3)	−0.016 (3)
C1B	0.047 (3)	0.063 (4)	0.074 (4)	−0.006 (3)	0.030 (3)	0.008 (3)
C2B	0.055 (4)	0.085 (5)	0.118 (7)	0.010 (4)	0.054 (5)	0.030 (5)
C3B	0.076 (5)	0.103 (7)	0.125 (8)	0.024 (5)	0.075 (6)	0.053 (6)
C4B	0.080 (5)	0.093 (6)	0.083 (5)	0.033 (4)	0.064 (4)	0.034 (4)
C5B	0.055 (4)	0.075 (4)	0.061 (4)	0.019 (3)	0.040 (3)	0.023 (3)
C6B	0.074 (4)	0.080 (5)	0.051 (3)	0.014 (4)	0.045 (3)	0.003 (3)

Geometric parameters (Å, º)

Cu—N1	1.980 (5)	N1B—C1B	1.360 (8)
Cu—N1B	1.980 (5)	C1—C2	1.455 (10)
Cu—N1A	1.984 (4)	C2—H21	0.9600
Cu—N	1.991 (5)	C2—H22	0.9600
Cu—O22A	2.379 (17)	C2—H23	0.9600
Cu—O22	2.455 (9)	C1A—C2A	1.380 (8)
Cu—O11	2.828 (5)	C1A—H1AA	0.9300

Cl1—O14A	1.317 (13)	C2A—C3A	1.360 (9)
Cl1—O12	1.387 (7)	C2A—H2AA	0.9300
Cl1—O13A	1.389 (13)	C3A—C4A	1.390 (9)
Cl1—O13	1.420 (7)	C3A—H3AA	0.9300
Cl1—O11	1.425 (5)	C4A—C5A	1.377 (8)
Cl1—O14	1.483 (8)	C4A—H4AA	0.9300
Cl1—O12A	1.524 (14)	C5A—C6A	1.503 (8)
Cl2—O24	1.394 (7)	C6A—H6AA	0.9700
Cl2—O21	1.406 (5)	C6A—H6AB	0.9700
Cl2—O23A	1.407 (13)	C1B—C2B	1.367 (9)
Cl2—O22A	1.412 (12)	C1B—H1BA	0.9300
Cl2—O22	1.428 (7)	C2B—C3B	1.403 (12)
Cl2—O24A	1.435 (12)	C2B—H2BA	0.9300
Cl2—O23	1.438 (7)	C3B—C4B	1.364 (12)
N—C6A	1.477 (8)	C3B—H3BA	0.9300
N—C6B	1.478 (7)	C4B—C5B	1.405 (8)
N—H0A	0.9100	C4B—H4BA	0.9300
N1—C1	1.137 (8)	C5B—C6B	1.512 (10)
N1A—C5A	1.341 (7)	C6B—H6BA	0.9700
N1A—C1A	1.344 (6)	C6B—H6BB	0.9700
N1B—C5B	1.320 (8)		

N1—Cu—N1B	97.2 (2)	C1A—N1A—Cu	126.2 (4)
N1—Cu—N1A	96.40 (19)	C5B—N1B—C1B	119.8 (5)
N1B—Cu—N1A	165.3 (2)	C5B—N1B—Cu	114.5 (4)
N1—Cu—N	175.1 (2)	C1B—N1B—Cu	125.6 (4)
N1B—Cu—N	83.0 (2)	N1—C1—C2	178.1 (8)
N1A—Cu—N	83.01 (19)	C1—C2—H21	109.5
N1—Cu—O22A	102.5 (9)	C1—C2—H22	109.5
N1B—Cu—O22A	85.3 (4)	H21—C2—H22	109.5
N1A—Cu—O22A	97.0 (5)	C1—C2—H23	109.5
N—Cu—O22A	82.4 (9)	H21—C2—H23	109.5
N1—Cu—O22	86.4 (4)	H22—C2—H23	109.5
N1B—Cu—O22	90.6 (3)	N1A—C1A—C2A	121.4 (6)
N1A—Cu—O22	95.6 (3)	N1A—C1A—H1AA	119.3
N—Cu—O22	98.5 (4)	C2A—C1A—H1AA	119.3
O22A—Cu—O22	16.4 (6)	C3A—C2A—C1A	119.0 (6)
N1—Cu—O11	87.9 (2)	C3A—C2A—H2AA	120.5
N1B—Cu—O11	80.84 (18)	C1A—C2A—H2AA	120.5
N1A—Cu—O11	94.23 (19)	C2A—C3A—C4A	120.0 (6)
N—Cu—O11	87.3 (2)	C2A—C3A—H3AA	120.0
O12—Cl1—O13	111.7 (6)	C4A—C3A—H3AA	120.0
O14A—Cl1—O11	116.3 (11)	C5A—C4A—C3A	118.4 (6)
O12—Cl1—O11	115.9 (5)	C5A—C4A—H4AA	120.8
O13A—Cl1—O11	107.6 (10)	C3A—C4A—H4AA	120.8
O13—Cl1—O11	112.9 (5)	N1A—C5A—C4A	121.5 (5)
O12—Cl1—O14	107.2 (6)	N1A—C5A—C6A	115.4 (5)
O13—Cl1—O14	102.8 (6)	C4A—C5A—C6A	123.1 (5)

O11—Cl1—O14	105.1 (5)	N—C6A—C5A	109.3 (5)
O14A—Cl1—O12A	107.3 (12)	N—C6A—H6AA	109.8
O13A—Cl1—O12A	104.8 (12)	C5A—C6A—H6AA	109.8
O24—Cl2—O21	113.2 (6)	N—C6A—H6AB	109.8
O21—Cl2—O23A	112.0 (11)	C5A—C6A—H6AB	109.8
O21—Cl2—O22A	112.0 (9)	H6AA—C6A—H6AB	108.3
O23A—Cl2—O22A	108.6 (10)	N1B—C1B—C2B	122.6 (7)
O24—Cl2—O22	110.2 (6)	N1B—C1B—H1BA	118.7
O21—Cl2—O22	111.8 (4)	C2B—C1B—H1BA	118.7
O21—Cl2—O24A	106.0 (10)	C1B—C2B—C3B	117.4 (8)
O23A—Cl2—O24A	109.1 (12)	C1B—C2B—H2BA	121.3
O22A—Cl2—O24A	108.9 (11)	C3B—C2B—H2BA	121.3
O24—Cl2—O23	108.6 (6)	C4B—C3B—C2B	120.2 (7)
O21—Cl2—O23	105.4 (5)	C4B—C3B—H3BA	119.9
O22—Cl2—O23	107.3 (5)	C2B—C3B—H3BA	119.9
Cl1—O11—Cu	155.4 (4)	C3B—C4B—C5B	119.1 (8)
Cl2—O22—Cu	124.0 (5)	C3B—C4B—H4BA	120.5
Cl2—O22A—Cu	130.1 (12)	C5B—C4B—H4BA	120.5
C6A—N—C6B	116.7 (5)	N1B—C5B—C4B	120.9 (7)
C6A—N—Cu	108.7 (4)	N1B—C5B—C6B	116.8 (5)
C6B—N—Cu	110.3 (4)	C4B—C5B—C6B	122.2 (7)
C6A—N—H0A	106.9	N—C6B—C5B	109.5 (5)
C6B—N—H0A	106.9	N—C6B—H6BA	109.8
Cu—N—H0A	106.9	C5B—C6B—H6BA	109.8
C1—N1—Cu	177.8 (6)	N—C6B—H6BB	109.8
C5A—N1A—C1A	119.6 (5)	C5B—C6B—H6BB	109.8
C5A—N1A—Cu	114.1 (3)	H6BA—C6B—H6BB	108.2

O14A—Cl1—O11—Cu	−174.7 (16)	O22—Cu—N1A—C5A	−109.8 (5)
O12—Cl1—O11—Cu	3.7 (12)	O11—Cu—N1A—C5A	74.8 (4)
O13A—Cl1—O11—Cu	−35.7 (16)	N1—Cu—N1A—C1A	−19.9 (5)
O13—Cl1—O11—Cu	134.3 (10)	N1B—Cu—N1A—C1A	−177.9 (7)
O14—Cl1—O11—Cu	−114.4 (10)	N—Cu—N1A—C1A	165.0 (5)
O12A—Cl1—O11—Cu	72.2 (14)	O22A—Cu—N1A—C1A	83.6 (10)
N1—Cu—O11—Cl1	152.0 (10)	O22—Cu—N1A—C1A	67.1 (6)
N1B—Cu—O11—Cl1	54.3 (10)	O11—Cu—N1A—C1A	−108.2 (5)
N1A—Cu—O11—Cl1	−111.8 (10)	N1—Cu—N1B—C5B	−161.1 (4)
N—Cu—O11—Cl1	−29.0 (10)	N1A—Cu—N1B—C5B	−3.1 (10)
O22A—Cu—O11—Cl1	22 (3)	N—Cu—N1B—C5B	14.0 (4)
O22—Cu—O11—Cl1	93 (2)	O22A—Cu—N1B—C5B	96.9 (10)
O24—Cl2—O22—Cu	−76.8 (8)	O22—Cu—N1B—C5B	112.5 (5)
O21—Cl2—O22—Cu	156.4 (6)	O11—Cu—N1B—C5B	−74.4 (4)
O23A—Cl2—O22—Cu	9.1 (16)	N1—Cu—N1B—C1B	17.1 (5)
O22A—Cl2—O22—Cu	60 (2)	N1A—Cu—N1B—C1B	175.0 (7)
O24A—Cl2—O22—Cu	−99.3 (11)	N—Cu—N1B—C1B	−167.9 (5)
O23—Cl2—O22—Cu	41.3 (8)	O22A—Cu—N1B—C1B	−85.0 (10)
N1—Cu—O22—Cl2	132.1 (10)	O22—Cu—N1B—C1B	−69.4 (6)
N1B—Cu—O22—Cl2	−130.7 (10)	O11—Cu—N1B—C1B	103.7 (5)

N1A—Cu—O22—Cl2	36.0 (10)	C5A—N1A—C1A—C2A	1.2 (9)
N—Cu—O22—Cl2	−47.7 (10)	Cu—N1A—C1A—C2A	−175.6 (4)
O22A—Cu—O22—Cl2	−59.7 (17)	N1A—C1A—C2A—C3A	−2.6 (10)
O11—Cu—O22—Cl2	−169.2 (11)	C1A—C2A—C3A—C4A	2.1 (10)
O24—Cl2—O22A—Cu	−21 (3)	C2A—C3A—C4A—C5A	−0.5 (9)
O21—Cl2—O22A—Cu	−171.5 (18)	C1A—N1A—C5A—C4A	0.5 (8)
O23A—Cl2—O22A—Cu	64 (2)	Cu—N1A—C5A—C4A	177.7 (4)
O22—Cl2—O22A—Cu	−76 (3)	C1A—N1A—C5A—C6A	178.4 (5)
O24A—Cl2—O22A—Cu	−55 (2)	Cu—N1A—C5A—C6A	−4.4 (6)
O23—Cl2—O22A—Cu	86 (2)	C3A—C4A—C5A—N1A	−0.9 (9)
N1—Cu—O22A—Cl2	83 (3)	C3A—C4A—C5A—C6A	−178.6 (6)
N1B—Cu—O22A—Cl2	180 (3)	C6B—N—C6A—C5A	−158.4 (5)
N1A—Cu—O22A—Cl2	−15 (3)	Cu—N—C6A—C5A	−32.9 (6)
N—Cu—O22A—Cl2	−97 (3)	N1A—C5A—C6A—N	25.0 (8)
O22—Cu—O22A—Cl2	71 (2)	C4A—C5A—C6A—N	−157.1 (6)
O11—Cu—O22A—Cl2	−148.2 (9)	C5B—N1B—C1B—C2B	1.1 (10)
N1B—Cu—N—C6A	−150.7 (4)	Cu—N1B—C1B—C2B	−177.0 (5)
N1A—Cu—N—C6A	25.0 (4)	N1B—C1B—C2B—C3B	0.6 (11)
O22A—Cu—N—C6A	123.1 (6)	C1B—C2B—C3B—C4B	−2.2 (11)
O22—Cu—N—C6A	119.7 (5)	C2B—C3B—C4B—C5B	2.2 (11)
O11—Cu—N—C6A	−69.6 (4)	C1B—N1B—C5B—C4B	−1.1 (9)
N1B—Cu—N—C6B	−21.5 (4)	Cu—N1B—C5B—C4B	177.1 (5)
N1A—Cu—N—C6B	154.2 (4)	C1B—N1B—C5B—C6B	178.8 (6)
O22A—Cu—N—C6B	−107.7 (6)	Cu—N1B—C5B—C6B	−3.0 (7)
O22—Cu—N—C6B	−111.1 (5)	C3B—C4B—C5B—N1B	−0.5 (10)
O11—Cu—N—C6B	59.6 (4)	C3B—C4B—C5B—C6B	179.6 (7)
N1—Cu—N1A—C5A	163.1 (4)	C6A—N—C6B—C5B	149.5 (6)
N1B—Cu—N1A—C5A	5.1 (10)	Cu—N—C6B—C5B	24.8 (6)
N—Cu—N1A—C5A	−12.0 (4)	N1B—C5B—C6B—N	−14.8 (8)
O22A—Cu—N1A—C5A	−93.4 (9)	C4B—C5B—C6B—N	165.2 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N—H0*A*···O22*A*	0.91	2.45	2.89 (3)	110
N—H0*A*···O23	0.91	2.30	3.084 (12)	144
N—H0*A*···O23^{i}	0.91	2.50	3.317 (10)	150
C2—H21···O13*A*^{ii}	0.96	2.23	2.98 (2)	133
C2—H22···O14^{iii}	0.96	2.36	3.103 (14)	134
C1*A*—H1*AA*···O12^{ii}	0.93	2.46	3.176 (9)	134
C3*A*—H3*AA*···O23^{iv}	0.93	2.53	3.376 (15)	152
C3*A*—H3*AA*···O23*A*^{iv}	0.93	2.29	2.993 (14)	133
C6*A*—H6*AA*···O21^{i}	0.97	2.56	3.381 (9)	143
C2*B*—H2*BA*···O14*A*^{v}	0.93	2.35	3.112 (16)	140
C3*B*—H3*BA*···O11^{vi}	0.93	2.56	3.429 (10)	156
C4*B*—H4*BA*···O24*A*^{vii}	0.93	2.25	3.06 (3)	145

C6*B*—H6*BA*···O12	0.97	2.56	3.425 (13)	149
C6*B*—H6*BB*···O24*A*^{vii}	0.97	2.51	3.211 (16)	129

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