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[(6-Methyl-2-pyridylmethyl)(2-pyridylmethyl)amine][(2-pyridylmethyl)amine]copper(II) bis(perchlorate)

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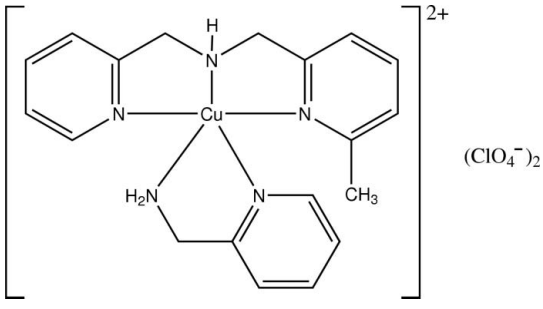
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.008 Å; disorder in solvent or counterion; R factor = 0.054; wR factor = 0.145; data-to-parameter ratio = 13.9.

The title compound, $[Cu(C_6H_8N_2)(C_{13}H_{15}N_3)](ClO_4)_2$, is a mixed ligand complex with the Cu^{II} atom coordinated by (6-methyl-2-pyridylmethyl)(2-pyridylmethyl)amine, acting as a tridentate ligand, and 2-(2-aminomethyl)pyridine, as a bidentate ligand, leading to an N_5 square-pyramidal geometry. The amine H atoms are involved in hydrogen bonding to the perchlorate O atoms and there are extensive but weak intermolecular C—H···O interactions in the crystal structure. The perchlorate ions are each disordered over two positions, with site occupancies of 0.601 (8):0.399 (8) and 0.659 (11):0.341 (11).

Related literature

For related literature, see: Cho *et al.* (2006); Gultneh *et al.* (2003); Hetterscheid *et al.* (2004); Mizuno *et al.* (2003); Ohtsu *et al.* (2001); Oki *et al.* (1990); Addison *et al.* (1984).



Experimental

Crystal data

$[Cu(C_6H_8N_2)(C_{13}H_{15}N_3)](ClO_4)_2$
M_r = 583.86
Monoclinic, $P2_1/n$
a = 9.3178 (10) Å
b = 13.9691 (19) Å
c = 19.223 (3) Å
β = 99.931 (11)°
V = 2464.6 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.16 mm^{-1}
T = 293 (2) K
0.45 × 0.22 × 0.17 mm

Data collection

Bruker $P4S$ diffractometer
Absorption correction: ψ-scan (North *et al.*, 1968)
T_{min} = 0.444, T_{max} = 0.505
(expected range = 0.722–0.821)
5832 measured reflections
5494 independent reflections
3410 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
3 standard reflections
every 97 reflections
intensity decay: < 2%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.145
S = 1.02
5494 reflections
394 parameters
118 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···O12A	0.90	2.21	3.080 (17)	161
N2—H2B···O13	0.90	2.27	3.103 (12)	154
N2—H2C···O24	0.90	2.22	3.064 (9)	157
N2—H2C···O22A	0.90	2.27	3.158 (19)	169
N2—H2C···O21	0.90	2.64	3.374 (17)	139
N—H0A···O12^{i}	0.91	2.44	3.301 (10)	158
N—H0A···O11A^{i}	0.91	2.40	3.291 (19)	165
C3—H3A···O23^{ii}	0.93	2.54	3.456 (10)	169
C4—H4A···O12^{iii}	0.93	2.45	3.374 (10)	172
C1A—H1AA···O14A	0.93	2.57	3.438 (18)	156
C2A—H2AA···O22^{iv}	0.93	2.56	3.475 (13)	167
C2A—H2AA···O22A^{iv}	0.93	2.46	3.199 (14)	136
C6A—H6AB···O22^{v}	0.97	2.35	3.294 (10)	164
C11B—H11B···O14A	0.96	2.32	3.180 (12)	148
C6B—H6BA···O22^{v}	0.97	2.53	3.433 (10)	154
C6B—H6BA···O23A^{v}	0.97	2.47	3.433 (17)	172
C6B—H6BB···O23^{vi}	0.97	2.54	3.375 (10)	144

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

Data collection: *XSCANS* (Bruker, 1997); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Bruker, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; 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: TK2224).

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supporting information

Acta Cryst. (2008). E**64**, m74–m75 [https://doi.org/10.1107/S1600536807062952]

[(6-Methyl-2-pyridylmethyl)(2-pyridylmethyl)amine][(2-pyridylmethyl)amine]-copper(II) bis(perchlorate)

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

S1. Comment

The geometry around the Cu^{II} ion in (I), Fig. 1, is best described as a distorted square-pyramid (τ = 0.224; Addison *et al.*, 1984), with an amine-N2 atom and three pyridine-N atoms (N1A, N1B, and N1) defining the basal plane. The Cu—$N_{pyridyl}$ bond distances are in the range of 1.993 (3)–2.039 (3) Å, and a Cu—N_{amine} bond distance of 1.998 (3) Å. The axial position is occupied by the amine-N atom of the tridentate (6-methyl-2-pyridylmethyl)(2-pyridylmethyl)amine ligand with a bond distance of 2.195 (3) Å consistent with a Jahn–Teller elongation. In (I), the Cu—$N_{pyridyl}$ and Cu—N_{amine} bond distances of 1.993 (3) and 1.998 (3) Å, respectively, are shorter for the 2-(2-aminomethyl)pyridine ligand. The amine H atoms are involved in hydrogen bonding to the perchlorate-O atoms and there are extensive but weak intermolecular C—H···O interactions in the crystal structure (Fig. 2 & Table 1).

S2. Experimental

Complex (I) was synthesized by reacting one equivalent each of the ligands (6-methyl-2-pyridylmethyl)(2-pyridyl-methyl)amine and 2-(2-aminomethyl)pyridine with $Cu(ClO_4)_2.6H_2O$ and triethylamine in methanol solution. After stirring the mixture for 12 h, the resulting precipitate was isolated and re-dissolved in acetonitrile solution. Dark-blue crystals suitable for X-ray diffraction analysis were obtained by layering this solution with diethyl ether.

S3. Refinement

The two perchlorate anions are disordered over two conformations with occupancy factors of 0.601 (8), 0.399 (8) for the Cl1-perchlorate anion, and 0.659 (11), 0.341 (11) for the Cl2-perchlorate. Each of the perchlorates was constrained to adopt a tetrahedral geometry. The H atoms were included in the riding model approximation with N—H = 0.90–0.91 Å and C—H = 0.93–0.97 Å, and with U_{iso}(H) = 1.2U_{eq}(C, N) (1.5U_{eq}(C) for methyl-H).

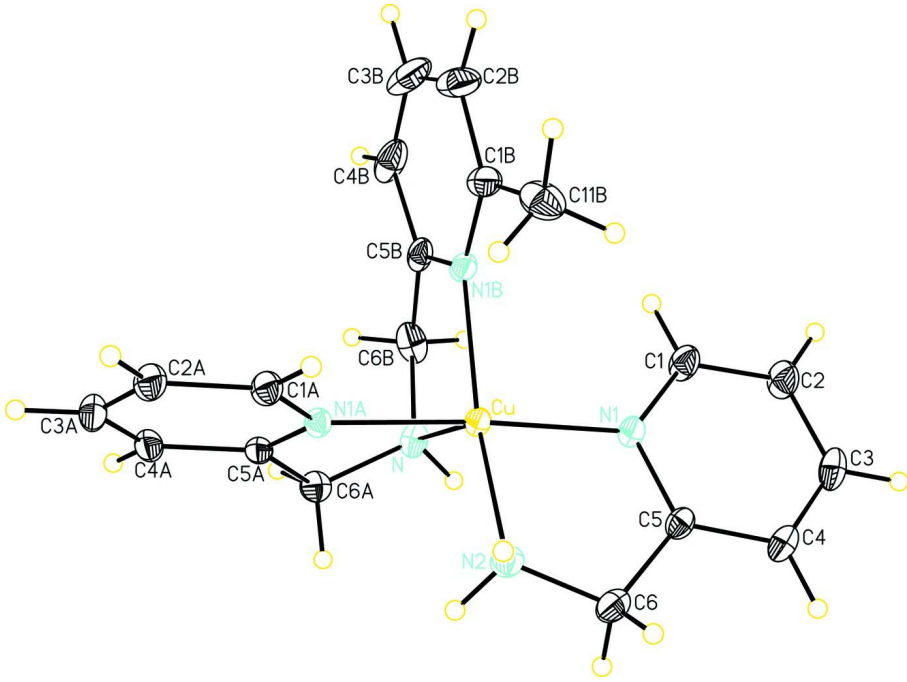

Figure 1

The molecular structure of (I) showing the atomic numbering scheme and displacement ellipsoids drawn at the 20% probabilty level.

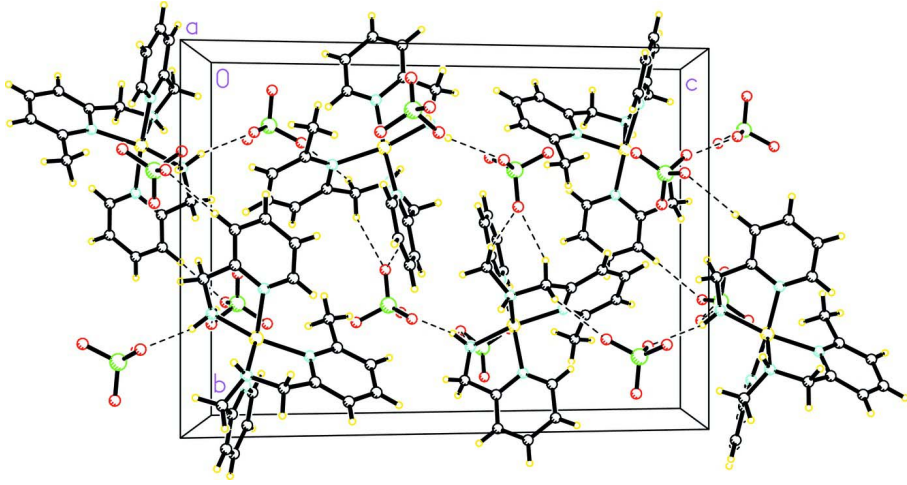

Figure 2

The packing arrangement in (I) viewed down the *a* axis showing the N—H···O and C—H···O interactions as dashed bonds.

[(6-Methyl-2-pyridylmethyl)(2-pyridylmethyl)amine][(2- pyridylmethyl)amine]copper(II) bis(perchlorate)

Crystal data

$[Cu(C_6H_8N_2)(C_{13}H_{15}N_3)](ClO_4)_2$
M_r = 583.86
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn

a = 9.3178 (10) Å
b = 13.9691 (19) Å
c = 19.223 (3) Å
β = 99.931 (11)°

V = 2464.6 (6) Å^3
Z = 4
F(000) = 1196
D_x = 1.574 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 40 reflections

θ = 5.1–12.5°
μ = 1.16 mm^{-1}
T = 293 K
Needle, dark blue
0.45 × 0.22 × 0.17 mm

Data collection

Bruker P4S diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: empirical (using intensity measurements) ψ-scan (North *et al.*, 1968)
T_{min} = 0.444, T_{max} = 0.505
5832 measured reflections

5494 independent reflections
3410 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 27.5°, θ_{min} = 2.6°
h = 0→10
k = 0→18
l = −24→24
3 standard reflections every 97 reflections
intensity decay: <2

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.145
S = 1.02
5494 reflections
394 parameters
118 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
$w = 1/[\sigma^2(F_o^2) + (0.0609P)^2 + 0.9236P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Cu	0.82061 (5)	0.75715 (3)	0.13019 (2)	0.05120 (17)	
Cl1	0.31446 (13)	0.67766 (9)	0.06898 (6)	0.0720 (3)	
Cl2	0.79982 (12)	0.81545 (7)	−0.12730 (6)	0.0641 (3)	
O11	0.3166 (9)	0.7331 (9)	0.1286 (5)	0.152 (4)	0.601 (8)
O12	0.1675 (7)	0.6764 (9)	0.0381 (6)	0.153 (4)	0.601 (8)
O13	0.3873 (12)	0.7307 (8)	0.0218 (5)	0.159 (4)	0.601 (8)
O14	0.3776 (16)	0.5943 (7)	0.0733 (8)	0.209 (5)	0.601 (8)
O11A	0.256 (2)	0.7538 (10)	0.0342 (10)	0.183 (6)	0.399 (8)
O12A	0.4019 (17)	0.6278 (13)	0.0278 (9)	0.175 (5)	0.399 (8)

O13A	0.2181 (16)	0.6067 (10)	0.0823 (9)	0.155 (5)	0.399 (8)
O14A	0.4133 (19)	0.6940 (15)	0.1287 (7)	0.194 (7)	0.399 (8)
O21	0.9137 (13)	0.7800 (12)	−0.0783 (7)	0.115 (4)	0.659 (11)
O22	0.7988 (12)	0.9139 (5)	−0.1336 (7)	0.135 (4)	0.659 (11)
O23	0.7929 (11)	0.7683 (7)	−0.1931 (3)	0.111 (3)	0.659 (11)
O24	0.6647 (8)	0.7921 (7)	−0.1036 (5)	0.124 (3)	0.659 (11)
O21A	0.941 (2)	0.780 (2)	−0.0915 (13)	0.114 (7)	0.341 (11)
O22A	0.735 (2)	0.8536 (14)	−0.0741 (7)	0.130 (5)	0.341 (11)
O23A	0.840 (3)	0.8895 (13)	−0.1687 (11)	0.152 (8)	0.341 (11)
O24A	0.728 (2)	0.7459 (10)	−0.1643 (11)	0.128 (6)	0.341 (11)
N1	0.9081 (4)	0.6274 (2)	0.14801 (18)	0.0582 (8)	
N2	0.7204 (4)	0.6948 (3)	0.04142 (19)	0.0711 (10)	
H2B	0.6256	0.6870	0.0439	0.085*	
H2C	0.7261	0.7336	0.0046	0.085*	
N	1.0124 (4)	0.8442 (3)	0.1207 (2)	0.0676 (10)	
H0A	1.0778	0.8088	0.1015	0.081*	
N1A	0.7231 (4)	0.8851 (2)	0.10460 (16)	0.0528 (8)	
C1	0.9991 (6)	0.5995 (4)	0.2061 (3)	0.0838 (15)	
H1A	1.0200	0.6419	0.2438	0.101*	
C2	1.0625 (6)	0.5108 (4)	0.2119 (3)	0.0928 (17)	
H2A	1.1239	0.4928	0.2532	0.111*	
C3	1.0343 (6)	0.4493 (4)	0.1563 (3)	0.0893 (16)	
H3A	1.0773	0.3890	0.1591	0.107*	
C4	0.9423 (5)	0.4767 (3)	0.0963 (3)	0.0747 (13)	
H4A	0.9213	0.4352	0.0581	0.090*	
C5	0.8813 (5)	0.5668 (3)	0.0934 (2)	0.0586 (10)	
C6	0.7826 (7)	0.6032 (4)	0.0292 (3)	0.0898 (16)	
H6A	0.8371	0.6090	−0.0093	0.108*	
H6B	0.7048	0.5574	0.0151	0.108*	
C1A	0.5863 (5)	0.9080 (3)	0.1121 (2)	0.0678 (12)	
H1AA	0.5272	0.8609	0.1264	0.081*	
C2A	0.5311 (6)	0.9987 (4)	0.0992 (3)	0.0824 (15)	
H2AA	0.4362	1.0128	0.1048	0.099*	
C3A	0.6177 (7)	1.0677 (4)	0.0780 (3)	0.0912 (17)	
H3AA	0.5820	1.1294	0.0688	0.109*	
C4A	0.7575 (6)	1.0460 (3)	0.0703 (2)	0.0750 (13)	
H4AA	0.8179	1.0927	0.0565	0.090*	
C5A	0.8077 (5)	0.9526 (3)	0.0835 (2)	0.0591 (10)	
C6A	0.9570 (5)	0.9222 (3)	0.0733 (2)	0.0691 (12)	
H6AA	0.9535	0.9019	0.0248	0.083*	
H6AB	1.0228	0.9764	0.0819	0.083*	
N1B	0.8682 (4)	0.8030 (2)	0.23229 (17)	0.0591 (9)	
C1B	0.7839 (6)	0.7840 (4)	0.2815 (3)	0.0811 (16)	
C11B	0.6648 (6)	0.7120 (5)	0.2627 (3)	0.105 (2)	
H11A	0.7063	0.6510	0.2546	0.158*	
H11B	0.6007	0.7322	0.2207	0.158*	
H11C	0.6108	0.7066	0.3008	0.158*	
C2B	0.8124 (8)	0.8284 (6)	0.3461 (3)	0.120 (3)	

H2BA	0.7582	0.8131	0.3808	0.145*
C3B	0.9221 (11)	0.8958 (7)	0.3591 (4)	0.146 (4)
H3BA	0.9395	0.9281	0.4020	0.175*
C4B	1.0036 (8)	0.9143 (4)	0.3092 (4)	0.116 (3)
H4BA	1.0768	0.9602	0.3174	0.139*
C5B	0.9783 (6)	0.8648 (3)	0.2458 (3)	0.0728 (14)
C6B	1.0765 (6)	0.8746 (4)	0.1921 (3)	0.0904 (17)
H6BA	1.1056	0.9411	0.1904	0.108*
H6BB	1.1638	0.8372	0.2076	0.108*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu	0.0506 (3)	0.0457 (3)	0.0560 (3)	0.0023 (2)	0.0057 (2)	−0.0030 (2)
Cl1	0.0659 (7)	0.0798 (8)	0.0700 (7)	−0.0029 (6)	0.0109 (6)	−0.0066 (6)
Cl2	0.0725 (7)	0.0507 (6)	0.0661 (6)	0.0027 (5)	0.0036 (5)	−0.0019 (5)
O11	0.095 (6)	0.257 (12)	0.103 (6)	0.002 (7)	0.011 (5)	−0.087 (7)
O12	0.062 (4)	0.198 (10)	0.191 (9)	−0.012 (5)	−0.003 (5)	−0.065 (8)
O13	0.164 (8)	0.168 (8)	0.166 (7)	−0.005 (7)	0.083 (7)	0.047 (7)
O14	0.248 (11)	0.127 (7)	0.258 (12)	0.083 (8)	0.063 (10)	0.051 (8)
O11A	0.175 (12)	0.153 (11)	0.226 (12)	0.070 (9)	0.045 (11)	0.080 (9)
O12A	0.165 (9)	0.185 (12)	0.205 (12)	0.053 (10)	0.115 (9)	0.029 (11)
O13A	0.127 (10)	0.128 (10)	0.227 (12)	−0.046 (8)	0.076 (9)	0.015 (9)
O14A	0.164 (13)	0.270 (17)	0.116 (10)	−0.105 (13)	−0.059 (10)	0.006 (11)
O21	0.113 (7)	0.134 (7)	0.084 (5)	0.029 (6)	−0.019 (5)	0.004 (5)
O22	0.132 (7)	0.053 (4)	0.210 (11)	−0.012 (4)	0.000 (7)	0.003 (5)
O23	0.129 (7)	0.125 (7)	0.073 (4)	0.017 (5)	0.001 (4)	−0.024 (4)
O24	0.098 (5)	0.107 (6)	0.175 (8)	−0.004 (4)	0.052 (5)	0.021 (5)
O21A	0.072 (9)	0.133 (12)	0.122 (14)	0.042 (9)	−0.021 (9)	−0.038 (11)
O22A	0.128 (11)	0.127 (11)	0.140 (10)	0.051 (9)	0.042 (8)	−0.022 (9)
O23A	0.200 (16)	0.091 (12)	0.168 (16)	−0.026 (11)	0.037 (12)	0.051 (11)
O24A	0.111 (11)	0.092 (8)	0.167 (13)	−0.025 (8)	−0.019 (9)	−0.045 (9)
N1	0.058 (2)	0.0481 (19)	0.067 (2)	0.0039 (16)	0.0069 (17)	−0.0052 (16)
N2	0.075 (2)	0.071 (2)	0.063 (2)	0.005 (2)	−0.0003 (19)	−0.0083 (19)
N	0.051 (2)	0.057 (2)	0.097 (3)	0.0004 (17)	0.020 (2)	−0.001 (2)
N1A	0.051 (2)	0.0505 (18)	0.0553 (19)	0.0033 (16)	0.0048 (15)	−0.0013 (15)
C1	0.084 (4)	0.069 (3)	0.088 (3)	0.026 (3)	−0.015 (3)	−0.013 (3)
C2	0.092 (4)	0.077 (4)	0.100 (4)	0.029 (3)	−0.009 (3)	0.001 (3)
C3	0.082 (4)	0.053 (3)	0.136 (5)	0.014 (3)	0.027 (4)	0.001 (3)
C4	0.072 (3)	0.055 (3)	0.099 (4)	0.000 (2)	0.023 (3)	−0.019 (3)
C5	0.054 (2)	0.051 (2)	0.072 (3)	−0.0076 (19)	0.016 (2)	−0.010 (2)
C6	0.115 (4)	0.071 (3)	0.077 (3)	0.012 (3)	0.001 (3)	−0.020 (3)
C1A	0.061 (3)	0.070 (3)	0.069 (3)	0.014 (2)	0.002 (2)	−0.001 (2)
C2A	0.076 (3)	0.086 (4)	0.080 (3)	0.032 (3)	−0.001 (3)	−0.004 (3)
C3A	0.120 (5)	0.061 (3)	0.085 (4)	0.029 (3)	−0.004 (3)	−0.001 (3)
C4A	0.100 (4)	0.054 (3)	0.066 (3)	0.002 (3)	0.000 (3)	0.005 (2)
C5A	0.074 (3)	0.053 (2)	0.047 (2)	0.001 (2)	−0.001 (2)	−0.0026 (18)
C6A	0.069 (3)	0.068 (3)	0.073 (3)	−0.013 (2)	0.017 (2)	0.001 (2)

N1B	0.065 (2)	0.054 (2)	0.056 (2)	0.0133 (18)	0.0019 (17)	−0.0060 (16)
C1B	0.082 (4)	0.100 (4)	0.060 (3)	0.047 (3)	0.008 (3)	0.001 (3)
C11B	0.087 (4)	0.142 (6)	0.095 (4)	0.010 (4)	0.037 (3)	0.025 (4)
C2B	0.125 (6)	0.174 (8)	0.061 (4)	0.084 (6)	0.012 (4)	−0.008 (4)
C3B	0.157 (8)	0.168 (8)	0.093 (5)	0.090 (7)	−0.029 (5)	−0.067 (6)
C4B	0.114 (5)	0.085 (4)	0.125 (5)	0.029 (4)	−0.048 (4)	−0.044 (4)
C5B	0.077 (3)	0.054 (3)	0.076 (3)	0.020 (2)	−0.021 (3)	−0.010 (2)
C6B	0.066 (3)	0.079 (4)	0.113 (4)	−0.016 (3)	−0.019 (3)	0.022 (3)

Geometric parameters (Å, º)

Cu—N1	1.993 (3)	C3—C4	1.367 (7)
Cu—N2	1.998 (3)	C3—H3A	0.9300
Cu—N1A	2.027 (3)	C4—C5	1.378 (6)
Cu—N1B	2.039 (3)	C4—H4A	0.9300
Cu—N	2.195 (3)	C5—C6	1.496 (7)
Cl1—O14	1.301 (9)	C6—H6A	0.9700
Cl1—O11A	1.321 (10)	C6—H6B	0.9700
Cl1—O14A	1.362 (10)	C1A—C2A	1.374 (6)
Cl1—O11	1.381 (7)	C1A—H1AA	0.9300
Cl1—O13A	1.391 (9)	C2A—C3A	1.364 (8)
Cl1—O12	1.396 (7)	C2A—H2AA	0.9300
Cl1—O12A	1.414 (11)	C3A—C4A	1.370 (7)
Cl1—O13	1.430 (7)	C3A—H3AA	0.9300
Cl2—O24A	1.315 (11)	C4A—C5A	1.394 (6)
Cl2—O22A	1.380 (10)	C4A—H4AA	0.9300
Cl2—O22	1.381 (7)	C5A—C6A	1.499 (6)
Cl2—O21	1.383 (8)	C6A—H6AA	0.9700
Cl2—O23A	1.396 (12)	C6A—H6AB	0.9700
Cl2—O23	1.417 (6)	N1B—C5B	1.332 (6)
Cl2—O24	1.448 (6)	N1B—C1B	1.356 (6)
Cl2—O21A	1.461 (13)	C1B—C2B	1.371 (8)
N1—C5	1.337 (5)	C1B—C11B	1.495 (8)
N1—C1	1.337 (6)	C11B—H11A	0.9600
N2—C6	1.440 (6)	C11B—H11B	0.9600
N2—H2B	0.9000	C11B—H11C	0.9600
N2—H2C	0.9000	C2B—C3B	1.380 (11)
N—C6A	1.456 (6)	C2B—H2BA	0.9300
N—C6B	1.462 (6)	C3B—C4B	1.347 (11)
N—H0A	0.9100	C3B—H3BA	0.9300
N1A—C5A	1.336 (5)	C4B—C5B	1.386 (7)
N1A—C1A	1.346 (5)	C4B—H4BA	0.9300
C1—C2	1.369 (7)	C5B—C6B	1.499 (7)
C1—H1A	0.9300	C6B—H6BA	0.9700
C2—C3	1.361 (7)	C6B—H6BB	0.9700
C2—H2A	0.9300		
N1—Cu—N2	82.37 (15)	C3—C4—C5	118.9 (5)

N1—Cu—N1A	175.43 (13)	C3—C4—H4A	120.5
N2—Cu—N1A	93.06 (14)	C5—C4—H4A	120.5
N1—Cu—N1B	96.05 (14)	N1—C5—C4	121.8 (4)
N2—Cu—N1B	161.97 (16)	N1—C5—C6	116.0 (4)
N1A—Cu—N1B	88.33 (13)	C4—C5—C6	122.3 (4)
N1—Cu—N	101.74 (14)	N2—C6—C5	112.0 (4)
N2—Cu—N	115.93 (16)	N2—C6—H6A	109.2
N1A—Cu—N	80.11 (13)	C5—C6—H6A	109.2
N1B—Cu—N	82.03 (15)	N2—C6—H6B	109.2
O11A—Cl1—O14A	116.7 (11)	C5—C6—H6B	109.2
O14—Cl1—O11	120.5 (8)	H6A—C6—H6B	107.9
O11A—Cl1—O13A	116.5 (10)	N1A—C1A—C2A	122.2 (5)
O14A—Cl1—O13A	109.2 (9)	N1A—C1A—H1AA	118.9
O14—Cl1—O12	114.6 (8)	C2A—C1A—H1AA	118.9
O11—Cl1—O12	103.5 (5)	C3A—C2A—C1A	118.9 (5)
O11A—Cl1—O12A	109.8 (10)	C3A—C2A—H2AA	120.6
O14A—Cl1—O12A	100.6 (10)	C1A—C2A—H2AA	120.6
O13A—Cl1—O12A	101.9 (9)	C2A—C3A—C4A	119.9 (5)
O12—Cl1—O12A	111.9 (9)	C2A—C3A—H3AA	120.1
O14—Cl1—O13	104.2 (7)	C4A—C3A—H3AA	120.1
O11—Cl1—O13	107.2 (7)	C3A—C4A—C5A	118.9 (5)
O12—Cl1—O13	105.9 (7)	C3A—C4A—H4AA	120.6
O24A—Cl2—O22A	116.2 (10)	C5A—C4A—H4AA	120.6
O24A—Cl2—O21	111.1 (12)	N1A—C5A—C4A	121.2 (4)
O22—Cl2—O21	114.2 (7)	N1A—C5A—C6A	116.7 (4)
O24A—Cl2—O23A	113.6 (11)	C4A—C5A—C6A	122.0 (4)
O22A—Cl2—O23A	109.3 (9)	N—C6A—C5A	111.5 (4)
O22—Cl2—O23	112.7 (6)	N—C6A—H6AA	109.3
O21—Cl2—O23	110.6 (7)	C5A—C6A—H6AA	109.3
O22—Cl2—O24	105.0 (5)	N—C6A—H6AB	109.3
O21—Cl2—O24	108.2 (7)	C5A—C6A—H6AB	109.3
O23—Cl2—O24	105.5 (5)	H6AA—C6A—H6AB	108.0
O24A—Cl2—O21A	109.3 (12)	C5B—N1B—C1B	120.6 (4)
O22A—Cl2—O21A	104.7 (11)	C5B—N1B—Cu	115.1 (3)
O23A—Cl2—O21A	102.4 (12)	C1B—N1B—Cu	123.7 (3)
C5—N1—C1	118.4 (4)	N1B—C1B—C2B	119.9 (6)
C5—N1—Cu	115.2 (3)	N1B—C1B—C11B	117.3 (4)
C1—N1—Cu	126.1 (3)	C2B—C1B—C11B	122.8 (6)
C6—N2—Cu	112.6 (3)	C1B—C11B—H11A	109.5
C6—N2—H2B	109.1	C1B—C11B—H11B	109.5
Cu—N2—H2B	109.1	H11A—C11B—H11B	109.5
C6—N2—H2C	109.1	C1B—C11B—H11C	109.5
Cu—N2—H2C	109.1	H11A—C11B—H11C	109.5
H2B—N2—H2C	107.8	H11B—C11B—H11C	109.5
C6A—N—C6B	114.4 (4)	C1B—C2B—C3B	119.6 (7)
C6A—N—Cu	105.1 (3)	C1B—C2B—H2BA	120.2
C6B—N—Cu	106.8 (3)	C3B—C2B—H2BA	120.2
C6A—N—H0A	110.1	C4B—C3B—C2B	119.5 (7)

C6B—N—H0A	110.1	C4B—C3B—H3BA	120.3
Cu—N—H0A	110.1	C2B—C3B—H3BA	120.3
C5A—N1A—C1A	118.9 (4)	C3B—C4B—C5B	119.9 (7)
C5A—N1A—Cu	115.6 (3)	C3B—C4B—H4BA	120.0
C1A—N1A—Cu	125.3 (3)	C5B—C4B—H4BA	120.0
N1—C1—C2	122.3 (5)	N1B—C5B—C4B	120.2 (6)
N1—C1—H1A	118.9	N1B—C5B—C6B	117.8 (4)
C2—C1—H1A	118.9	C4B—C5B—C6B	121.9 (6)
C3—C2—C1	119.0 (5)	N—C6B—C5B	114.9 (4)
C3—C2—H2A	120.5	N—C6B—H6BA	108.5
C1—C2—H2A	120.5	C5B—C6B—H6BA	108.5
C2—C3—C4	119.6 (5)	N—C6B—H6BB	108.5
C2—C3—H3A	120.2	C5B—C6B—H6BB	108.5
C4—C3—H3A	120.2	H6BA—C6B—H6BB	107.5

N2—Cu—N1—C5	9.1 (3)	C5A—N1A—C1A—C2A	−0.4 (6)
N1A—Cu—N1—C5	7.6 (19)	Cu—N1A—C1A—C2A	174.5 (3)
N1B—Cu—N1—C5	171.0 (3)	N1A—C1A—C2A—C3A	0.1 (7)
N—Cu—N1—C5	−105.9 (3)	C1A—C2A—C3A—C4A	−0.4 (8)
N2—Cu—N1—C1	−177.1 (4)	C2A—C3A—C4A—C5A	0.9 (7)
N1A—Cu—N1—C1	−179 (36)	C1A—N1A—C5A—C4A	1.0 (6)
N1B—Cu—N1—C1	−15.1 (4)	Cu—N1A—C5A—C4A	−174.4 (3)
N—Cu—N1—C1	67.9 (4)	C1A—N1A—C5A—C6A	−177.6 (4)
N1—Cu—N2—C6	−12.6 (4)	Cu—N1A—C5A—C6A	7.0 (4)
N1A—Cu—N2—C6	167.3 (4)	C3A—C4A—C5A—N1A	−1.2 (7)
N1B—Cu—N2—C6	−98.7 (6)	C3A—C4A—C5A—C6A	177.3 (4)
N—Cu—N2—C6	86.8 (4)	C6B—N—C6A—C5A	−81.9 (5)
N1—Cu—N—C6A	150.8 (3)	Cu—N—C6A—C5A	34.9 (4)
N2—Cu—N—C6A	63.7 (3)	N1A—C5A—C6A—N	−30.2 (5)
N1A—Cu—N—C6A	−24.9 (3)	C4A—C5A—C6A—N	151.2 (4)
N1B—Cu—N—C6A	−114.6 (3)	N1—Cu—N1B—C5B	105.0 (3)
N1—Cu—N—C6B	−87.2 (3)	N2—Cu—N1B—C5B	−171.0 (4)
N2—Cu—N—C6B	−174.4 (3)	N1A—Cu—N1B—C5B	−76.3 (3)
N1A—Cu—N—C6B	97.0 (3)	N—Cu—N1B—C5B	4.0 (3)
N1B—Cu—N—C6B	7.3 (3)	N1—Cu—N1B—C1B	−84.0 (4)
N1—Cu—N1A—C5A	−103.9 (17)	N2—Cu—N1B—C1B	0.0 (7)
N2—Cu—N1A—C5A	−105.4 (3)	N1A—Cu—N1B—C1B	94.7 (3)
N1B—Cu—N1A—C5A	92.6 (3)	N—Cu—N1B—C1B	174.9 (4)
N—Cu—N1A—C5A	10.4 (3)	C5B—N1B—C1B—C2B	−0.4 (7)
N1—Cu—N1A—C1A	81.0 (18)	Cu—N1B—C1B—C2B	−170.9 (4)
N2—Cu—N1A—C1A	79.6 (3)	C5B—N1B—C1B—C11B	−178.6 (4)
N1B—Cu—N1A—C1A	−82.4 (3)	Cu—N1B—C1B—C11B	10.9 (6)
N—Cu—N1A—C1A	−164.6 (3)	N1B—C1B—C2B—C3B	3.4 (9)
C5—N1—C1—C2	−1.5 (8)	C11B—C1B—C2B—C3B	−178.5 (6)
Cu—N1—C1—C2	−175.2 (4)	C1B—C2B—C3B—C4B	−2.7 (11)
N1—C1—C2—C3	1.2 (9)	C2B—C3B—C4B—C5B	−0.9 (11)
C1—C2—C3—C4	−0.8 (9)	C1B—N1B—C5B—C4B	−3.2 (6)
C2—C3—C4—C5	0.6 (8)	Cu—N1B—C5B—C4B	168.1 (4)

C1—N1—C5—C4	1.4 (6)	C1B—N1B—C5B—C6B	173.7 (4)
Cu—N1—C5—C4	175.7 (3)	Cu—N1B—C5B—C6B	−15.0 (5)
C1—N1—C5—C6	−178.1 (5)	C3B—C4B—C5B—N1B	3.9 (8)
Cu—N1—C5—C6	−3.7 (5)	C3B—C4B—C5B—C6B	−172.9 (6)
C3—C4—C5—N1	−0.9 (7)	C6A—N—C6B—C5B	99.2 (5)
C3—C4—C5—C6	178.5 (5)	Cu—N—C6B—C5B	−16.7 (5)
Cu—N2—C6—C5	13.8 (6)	N1B—C5B—C6B—N	22.1 (6)
N1—C5—C6—N2	−6.8 (7)	C4B—C5B—C6B—N	−161.0 (4)
C4—C5—C6—N2	173.8 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*B*···O12*A*	0.90	2.21	3.080 (17)	161
N2—H2*B*···O13	0.90	2.27	3.103 (12)	154
N2—H2*C*···O24	0.90	2.22	3.064 (9)	157
N2—H2*C*···O22*A*	0.90	2.27	3.158 (19)	169
N2—H2*C*···O21	0.90	2.64	3.374 (17)	139
N—H0*A*···O12^{i}	0.91	2.44	3.301 (10)	158
N—H0*A*···O11*A*^{i}	0.91	2.40	3.291 (19)	165
C3—H3*A*···O23^{ii}	0.93	2.54	3.456 (10)	169
C4—H4*A*···O12^{iii}	0.93	2.45	3.374 (10)	172
C1*A*—H1*AA*···O14*A*	0.93	2.57	3.438 (18)	156
C2*A*—H2*AA*···O22^{iv}	0.93	2.56	3.475 (13)	167
C2*A*—H2*AA*···O22*A*^{iv}	0.93	2.46	3.199 (14)	136
C6*A*—H6*AB*···O22^{v}	0.97	2.35	3.294 (10)	164
C11*B*—H11*B*···O14*A*	0.96	2.32	3.180 (12)	148
C6*B*—H6*BA*···O22^{v}	0.97	2.53	3.433 (10)	154
C6*B*—H6*BA*···O23*A*^{v}	0.97	2.47	3.433 (17)	172
C6*B*—H6*BB*···O23^{vi}	0.97	2.54	3.375 (10)	144

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) −*x*+2, −*y*+1, −*z*; (iii) −*x*+1, −*y*+1, −*z*; (iv) −*x*+1, −*y*+2, −*z*; (v) −*x*+2, −*y*+2, −*z*; (vi) *x*+1/2, −*y*+3/2, *z*+1/2.