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Chloridotetrakis(1-ethyl-1*H*-imidazole-κN^3)copper(II) chloride monohydrate

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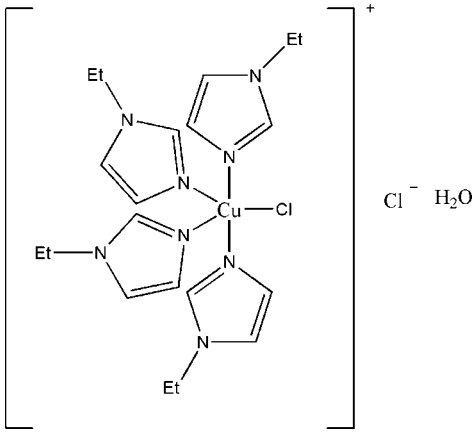
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.056; wR factor = 0.140; data-to-parameter ratio = 9.3.

The title compound, $[CuCl(C_5H_8N_2)_4]Cl\cdot H_2O$, consists of a discrete $[CuCl(Eim)_4]^+$ cation (Eim is 1-ethyl-1*H*-imidazole), one Cl^- anion and one water molecule. The Cu^{II} ion adopts a distorted square-pyramidal geometry. The basal coordination positions are occupied by the N atoms of the Eim ligands and the apical position is occupied by a Cl^- anion. In the crystal structure, ions and water molecules form three-dimensional hydrogen-bond networks which stabilize the structure.

Related literature

For related literature, see: Jian *et al.* (2004); Otieno *et al.* (2001).



Experimental

Crystal data

$[CuCl(C_5H_8N_2)_4]Cl\cdot H_2O$
M_r = 537.00
Monoclinic, *Cc*
a = 20.304 (4) Å
b = 8.6090 (17) Å
c = 17.364 (4) Å
β = 119.65 (3)°
V = 2637.8 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.06 mm^{-1}
T = 293 (2) K
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.816, T_{max} = 0.902
5104 measured reflections
2811 independent reflections
2013 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.140
S = 0.95
2811 reflections
302 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.77 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}
Absolute structure: Flack (1983), with 212 Friedel pairs
Flack parameter: 0.09 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···Cl2^{i}	0.84 (10)	2.47 (11)	3.206 (11)	147
O1W—H1WB···Cl1	0.85 (10)	2.39 (9)	3.183 (9)	156 (9)
C6—H6A···Cl2	0.93	2.61	3.401 (5)	143
C7—H7A···Cl2^{ii}	0.93	2.81	3.595 (6)	143
C9—H9B···Cl1^{iii}	0.97	2.72	3.598 (9)	151
C11—H11A···O1W^{iii}	0.93	2.47	3.361 (9)	161
C19—H19B···Cl1^{iv}	0.97	2.77	3.713 (12)	162

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and local programs.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2282).

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supplementary materials

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Chloridotetrakis(1-ethyl-1*H*-imidazole-κN^3)copper(II) chloride monohydrate

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Comment

In title compound, the crystal structure consists of discrete $CuCl(Eim)_4^+$ cations, Cl^- anions and water molecules. The Cu^{II} ion adopts a distorted square pyramidal geometry. The basal coordination positions are occupied by the N atoms of the Eim ligands with bond lengths ranging from 1.960 (7) to 2.075 (8) Å, and the apical position by a Cl anion [Cu—Cl = 2.730 (3) Å], while another chloride anion in the general position balances the charges. All these values agree well with two polymorphism complexes $[CuCl(im)_4Cl]$(im is 1*H*-imidazole) (Otieno *et al.*, 2001; Jian *et al.*, 2004). In the crystal, the title compound form three-dimensional hydrogen bond networks to stabilize the structure.

Experimental

The title compound was prepared by the reaction of 1-ethylimidazole (1.92 g, 20 mmol) with $CuCl_2{\cdot}2H_2O$ (0.68 g, 5 mmol) by means of hydrothermal synthesis in a stainless-steel reactor with Teflon liner at 383 K for 24 h. Single crystals suitable for X-ray measurements were obtained by recrystallization from ethanol at room temperature.

Refinement

H atoms bonded to O were located in a difference map and their coordinates were refined with U_{iso}(H)=1.2U_{eq}(O). The other H atoms were positioned geometrically (C—H = 0.93 Å) and allowed to ride on their attached atoms U_{iso}(H) = 1.2–1.5U_{eq}(C).

Figures

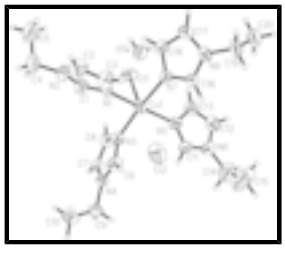


Fig. 1. The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

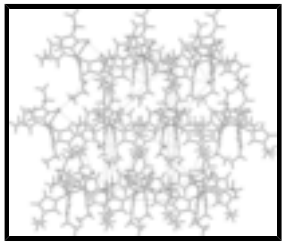


Fig. 2. The packing of (I), viewed down the *c* axis.

Chloridotetrakis(1-ethyl-1*H*-imidazole-κN^3)copper(II) chloride monohydrate

Crystal data

$[CuCl(C_5H_8N_2)_4]Cl·H_2O$	F_{000} = 1124
M_r = 537.00	D_x = 1.352 Mg m^{-3}
Monoclinic, *Cc*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: C -2yc	Cell parameters from 3489 reflections
a = 20.304 (4) Å	θ = 2.1–26.0º
b = 8.6090 (17) Å	μ = 1.06 mm^{-1}
c = 17.364 (4) Å	*T* = 293 (2) K
β = 119.65 (3)º	Block, blue
V = 2637.8 (12) Å^3	0.20 × 0.10 × 0.10 mm
Z = 4	

Data collection

Bruker SMART 1K CCD area-detector diffractometer	2811 independent reflections
Radiation source: fine-focus sealed tube	2013 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.022
T = 293(2) K	θ_{max} = 26.0º
thin–slice ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	*h* = −21→25
T_{min} = 0.816, T_{max} = 0.902	*k* = 0→10
5104 measured reflections	*l* = −21→0

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.056	$w = 1/[\sigma^2(F_o^2) + (0.0852P)^2 + 0.8132P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.140	$(\Delta/\sigma)_{max}$ = 0.007
S = 0.95	$\Delta\rho_{max}$ = 0.77 e Å^{-3}
2811 reflections	$\Delta\rho_{min}$ = −0.48 e Å^{-3}
302 parameters	Extinction correction: SHELXTL (Sheldrick, 2001), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
6 restraints	Extinction coefficient: 0.0042 (6)
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), with 212 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.09 (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	0.45278 (5)	0.93673 (12)	−0.00119 (6)	0.0418 (3)
Cl1	0.33081 (13)	0.7876 (3)	−0.13405 (17)	0.0541 (7)
Cl2	0.6087 (2)	1.1185 (3)	0.1607 (2)	0.0711 (9)
O1W	0.2390 (5)	0.6153 (12)	−0.3198 (5)	0.074 (2)
N1	0.3969 (4)	0.9903 (9)	0.0603 (5)	0.0382 (16)
N2	0.3177 (5)	0.9711 (11)	0.1131 (6)	0.054 (2)
N3	0.4954 (4)	0.7458 (8)	0.0708 (5)	0.0396 (17)
N4	0.5781 (4)	0.5894 (8)	0.1720 (4)	0.0358 (16)
N5	0.5177 (4)	0.9008 (10)	−0.0617 (5)	0.0402 (18)
N6	0.6119 (4)	0.8808 (10)	−0.0866 (6)	0.050 (2)
N7	0.4203 (4)	1.1413 (8)	−0.0680 (5)	0.0379 (17)
N8	0.4220 (4)	1.3575 (8)	−0.1323 (5)	0.0427 (18)
C1	0.3511 (2)	0.8971 (3)	0.0729 (2)	0.059 (3)
H1A	0.3429	0.7932	0.0561	0.070*
C2	0.3413 (2)	1.1234 (3)	0.1246 (2)	0.060 (3)
H2A	0.3266	1.2036	0.1488	0.073*
C3	0.3899 (2)	1.1316 (3)	0.0935 (2)	0.054 (3)
H3A	0.4158	1.2212	0.0942	0.065*
C4	0.2617 (2)	0.9038 (3)	0.1347 (2)	0.084 (4)
H4A	0.2658	0.7915	0.1361	0.100*
H4B	0.2731	0.9385	0.1932	0.100*
C5	0.1842 (2)	0.948 (2)	0.0704 (2)	0.103 (6)
H5A	0.1494	0.8758	0.0729	0.154*
H5B	0.1782	0.9481	0.0120	0.154*
H5C	0.1741	1.0506	0.0841	0.154*
C6	0.5594 (5)	0.7375 (3)	0.1456 (2)	0.045 (2)
H6A	0.5883	0.8232	0.1765	0.054*
C7	0.5227 (5)	0.4971 (3)	0.1093 (6)	0.0364 (18)
H7A	0.5202	0.3893	0.1092	0.044*
C8	0.4722 (5)	0.5951 (3)	0.0473 (6)	0.040 (2)
H8A	0.4282	0.5649	−0.0036	0.048*
C9	0.6465 (5)	0.5343 (3)	0.2516 (2)	0.052 (2)
H9A	0.6568	0.4284	0.2415	0.063*

H9B	0.6892	0.5977	0.2604	0.063*
C10	0.6412 (2)	0.5384 (3)	0.3314 (2)	0.083 (4)
H10A	0.6893	0.5115	0.3812	0.125*
H10B	0.6035	0.4655	0.3264	0.125*
H10C	0.6272	0.6410	0.3395	0.125*
C11	0.5895 (5)	0.8847 (3)	−0.0262 (2)	0.047 (2)
H11A	0.6222	0.8768	0.0345	0.056*
C12	0.5497 (2)	0.8989 (3)	−0.1665 (2)	0.056 (3)
H12A	0.5476	0.9031	−0.2212	0.067*
C13	0.4905 (2)	0.9099 (3)	−0.1509 (2)	0.054 (3)
H13A	0.4399	0.9216	−0.1939	0.065*
C14	0.6896 (2)	0.8680 (3)	−0.0699 (2)	0.084 (4)
H14A	0.6883	0.8400	−0.1248	0.101*
H14B	0.7148	0.7847	−0.0278	0.101*
C15	0.7343 (2)	1.0112 (3)	−0.0352 (2)	0.139 (8)
H15A	0.7862	0.9907	−0.0180	0.208*
H15B	0.7311	1.0466	0.0153	0.208*
H15C	0.7146	1.0898	−0.0803	0.208*
C16	0.4634 (5)	1.2435 (3)	−0.0789 (6)	0.042 (2)
H16A	0.5158	1.2366	−0.0526	0.051*
C17	0.3478 (2)	1.3303 (3)	−0.1580 (3)	0.050 (2)
H17A	0.3062	1.3907	−0.1955	0.059*
C18	0.3478 (5)	1.1944 (3)	−0.1164 (6)	0.046 (2)
H18A	0.3051	1.1464	−0.1206	0.056*
C19	0.4487 (7)	1.4891 (3)	−0.1631 (7)	0.057 (3)
H19A	0.5032	1.4987	−0.1261	0.069*
H19B	0.4257	1.5840	−0.1572	0.069*
C20	0.4292 (2)	1.4693 (3)	−0.2577 (3)	0.077 (4)
H20A	0.4537	1.5490	−0.2732	0.115*
H20B	0.3753	1.4770	−0.2955	0.115*
H20C	0.4462	1.3692	−0.2653	0.115*
H1WB	0.275 (5)	0.649 (18)	−0.271 (4)	0.11 (6)*
H1WA	0.202 (4)	0.587 (13)	−0.314 (7)	0.07 (4)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0530 (6)	0.0326 (5)	0.0509 (6)	0.0144 (6)	0.0343 (5)	0.0132 (6)
Cl1	0.0377 (12)	0.0500 (15)	0.0566 (15)	0.0011 (11)	0.0096 (11)	−0.0051 (12)
Cl2	0.108 (2)	0.0346 (13)	0.088 (2)	0.0124 (14)	0.0623 (19)	0.0071 (13)
O1W	0.052 (5)	0.105 (7)	0.056 (5)	−0.017 (5)	0.019 (4)	0.000 (5)
N1	0.040 (4)	0.039 (4)	0.045 (4)	0.003 (4)	0.029 (3)	0.010 (4)
N2	0.058 (5)	0.069 (6)	0.053 (5)	0.013 (5)	0.043 (5)	0.007 (5)
N3	0.043 (4)	0.037 (4)	0.037 (4)	0.002 (3)	0.018 (4)	−0.001 (3)
N4	0.035 (4)	0.032 (4)	0.034 (4)	−0.002 (3)	0.012 (3)	0.004 (3)
N5	0.041 (4)	0.044 (4)	0.037 (4)	0.014 (4)	0.021 (4)	−0.001 (4)
N6	0.041 (4)	0.053 (5)	0.055 (5)	0.003 (4)	0.024 (4)	−0.001 (4)
N7	0.040 (4)	0.031 (4)	0.047 (4)	0.005 (3)	0.025 (4)	0.002 (3)

N8	0.060 (5)	0.030 (4)	0.042 (4)	0.004 (3)	0.028 (4)	0.006 (3)
C1	0.072 (7)	0.048 (6)	0.073 (7)	0.009 (5)	0.050 (6)	0.018 (5)
C2	0.064 (6)	0.065 (7)	0.054 (6)	0.007 (6)	0.030 (6)	−0.015 (5)
C3	0.057 (6)	0.056 (6)	0.056 (6)	−0.015 (5)	0.033 (5)	−0.025 (5)
C4	0.109 (11)	0.079 (9)	0.107 (11)	0.011 (8)	0.088 (10)	0.024 (8)
C5	0.066 (9)	0.161 (19)	0.086 (10)	−0.015 (9)	0.042 (8)	0.005 (10)
C6	0.036 (5)	0.035 (5)	0.057 (6)	−0.002 (4)	0.017 (5)	−0.010 (5)
C7	0.040 (4)	0.027 (4)	0.043 (5)	−0.001 (4)	0.021 (4)	−0.003 (4)
C8	0.043 (5)	0.041 (5)	0.028 (4)	−0.015 (4)	0.011 (4)	−0.011 (4)
C9	0.041 (5)	0.054 (6)	0.047 (6)	0.007 (4)	0.012 (4)	0.011 (5)
C10	0.062 (7)	0.124 (13)	0.048 (7)	0.017 (8)	0.016 (6)	0.026 (8)
C11	0.032 (5)	0.061 (6)	0.044 (5)	0.004 (4)	0.017 (4)	0.002 (5)
C12	0.075 (8)	0.053 (7)	0.046 (6)	0.008 (5)	0.036 (6)	0.001 (5)
C13	0.062 (6)	0.058 (6)	0.044 (5)	0.014 (5)	0.029 (5)	0.006 (5)
C14	0.081 (9)	0.082 (9)	0.113 (11)	0.000 (7)	0.066 (9)	0.001 (8)
C15	0.085 (11)	0.106 (12)	0.24 (3)	−0.042 (10)	0.096 (15)	−0.025 (17)
C16	0.038 (5)	0.046 (5)	0.044 (5)	0.009 (4)	0.021 (4)	0.011 (4)
C17	0.047 (5)	0.045 (6)	0.052 (6)	0.014 (5)	0.021 (5)	0.010 (5)
C18	0.038 (5)	0.046 (5)	0.057 (6)	0.003 (4)	0.025 (5)	0.006 (5)
C19	0.089 (8)	0.036 (5)	0.070 (7)	0.000 (5)	0.058 (6)	0.007 (5)
C20	0.094 (9)	0.079 (9)	0.080 (8)	0.013 (7)	0.060 (8)	0.028 (7)

Geometric parameters (Å, °)

Cu1—N1	1.960 (7)	C5—H5A	0.9600
Cu1—N3	1.986 (7)	C5—H5B	0.9600
Cu1—N7	2.031 (7)	C5—H5C	0.9600
Cu1—N5	2.075 (8)	C6—H6A	0.9300
Cu1—Cl1	2.730 (3)	C7—C8	1.353 (13)
O1W—H1WB	0.85 (10)	C7—H7A	0.9300
O1W—H1WA	0.84 (10)	C8—H8A	0.9300
N1—C1	1.327 (13)	C9—C10	1.442 (7)
N1—C3	1.383 (13)	C9—H9A	0.9700
N2—C1	1.348 (13)	C9—H9B	0.9700
N2—C2	1.377 (15)	C10—H10A	0.9600
N2—C4	1.480 (14)	C10—H10B	0.9600
N3—C6	1.308 (12)	C10—H10C	0.9600
N3—C8	1.372 (11)	C11—H11A	0.9300
N4—C6	1.345 (11)	C12—C13	1.360 (6)
N4—C7	1.368 (11)	C12—H12A	0.9300
N4—C9	1.471 (12)	C13—H13A	0.9300
N5—C11	1.279 (11)	C14—C15	1.472 (4)
N5—C13	1.366 (13)	C14—H14A	0.9700
N6—C11	1.334 (13)	C14—H14B	0.9700
N6—C12	1.346 (14)	C15—H15A	0.9600
N6—C14	1.459 (14)	C15—H15B	0.9600
N7—C16	1.318 (11)	C15—H15C	0.9600
N7—C18	1.364 (11)	C16—H16A	0.9300
N8—C16	1.326 (11)	C17—C18	1.375 (6)

N8—C17	1.363 (12)	C17—H17A	0.9300
N8—C19	1.465 (12)	C18—H18A	0.9300
C1—H1A	0.9300	C19—C20	1.499 (17)
C2—C3	1.341 (6)	C19—H19A	0.9700
C2—H2A	0.9300	C19—H19B	0.9700
C3—H3A	0.9300	C20—H20A	0.9600
C4—C5	1.459 (7)	C20—H20B	0.9600
C4—H4A	0.9700	C20—H20C	0.9600
C4—H4B	0.9700		
N1—Cu1—N3	92.4 (3)	C8—C7—H7A	127.1
N1—Cu1—N7	89.8 (3)	N4—C7—H7A	127.1
N3—Cu1—N7	174.0 (3)	C7—C8—N3	109.8 (7)
N1—Cu1—N5	174.3 (4)	C7—C8—H8A	125.1
N3—Cu1—N5	90.4 (3)	N3—C8—H8A	125.1
N7—Cu1—N5	87.0 (3)	C10—C9—N4	114.2 (9)
N1—Cu1—Cl1	92.5 (2)	C10—C9—H9A	108.7
N3—Cu1—Cl1	94.2 (2)	N4—C9—H9A	108.7
N7—Cu1—Cl1	91.3 (2)	C10—C9—H9B	108.7
N5—Cu1—Cl1	92.3 (2)	N4—C9—H9B	108.7
H1WB—O1W—H1WA	111 (10)	H9A—C9—H9B	107.6
C1—N1—C3	103.8 (8)	C9—C10—H10A	109.5
C1—N1—Cu1	126.2 (7)	C9—C10—H10B	109.5
C3—N1—Cu1	129.8 (6)	H10A—C10—H10B	109.5
C1—N2—C2	107.4 (9)	C9—C10—H10C	109.5
C1—N2—C4	126.3 (10)	H10A—C10—H10C	109.5
C2—N2—C4	126.2 (10)	H10B—C10—H10C	109.5
C6—N3—C8	105.7 (8)	N5—C11—N6	112.0 (9)
C6—N3—Cu1	125.4 (6)	N5—C11—H11A	124.0
C8—N3—Cu1	128.1 (6)	N6—C11—H11A	124.0
C6—N4—C7	107.3 (7)	N6—C12—C13	105.9 (9)
C6—N4—C9	127.0 (7)	N6—C12—H12A	127.0
C7—N4—C9	125.7 (7)	C13—C12—H12A	127.0
C11—N5—C13	106.1 (9)	C12—C13—N5	108.7 (9)
C11—N5—Cu1	129.0 (7)	C12—C13—H13A	125.6
C13—N5—Cu1	124.4 (6)	N5—C13—H13A	125.6
C11—N6—C12	107.2 (8)	N6—C14—C15	113.9 (4)
C11—N6—C14	127.0 (10)	N6—C14—H14A	108.8
C12—N6—C14	125.7 (10)	C15—C14—H14A	108.8
C16—N7—C18	106.2 (8)	N6—C14—H14B	108.8
C16—N7—Cu1	127.6 (6)	C15—C14—H14B	108.8
C18—N7—Cu1	126.1 (6)	H14A—C14—H14B	107.7
C16—N8—C17	108.5 (8)	C14—C15—H15A	109.5
C16—N8—C19	127.3 (8)	C14—C15—H15B	109.5
C17—N8—C19	124.1 (8)	H15A—C15—H15B	109.5
N1—C1—N2	111.9 (9)	C14—C15—H15C	109.5
N1—C1—H1A	124.1	H15A—C15—H15C	109.5
N2—C1—H1A	124.1	H15B—C15—H15C	109.5
C3—C2—N2	105.3 (9)	N7—C16—N8	111.0 (8)
C3—C2—H2A	127.4	N7—C16—H16A	124.5

N2—C2—H2A	127.4	N8—C16—H16A	124.5
C2—C3—N1	111.7 (4)	N8—C17—C18	105.2 (8)
C2—C3—H3A	124.2	N8—C17—H17A	127.4
N1—C3—H3A	124.2	C18—C17—H17A	127.4
C5—C4—N2	112.1 (11)	N7—C18—C17	109.2 (8)
C5—C4—H4A	109.2	N7—C18—H18A	125.4
N2—C4—H4A	109.2	C17—C18—H18A	125.4
C5—C4—H4B	109.2	N8—C19—C20	111.5 (9)
N2—C4—H4B	109.2	N8—C19—H19A	109.3
H4A—C4—H4B	107.9	C20—C19—H19A	109.3
C4—C5—H5A	109.5	N8—C19—H19B	109.3
C4—C5—H5B	109.5	C20—C19—H19B	109.3
H5A—C5—H5B	109.5	H19A—C19—H19B	108.0
C4—C5—H5C	109.5	C19—C20—H20A	109.5
H5A—C5—H5C	109.5	C19—C20—H20B	109.5
H5B—C5—H5C	109.5	H20A—C20—H20B	109.5
N3—C6—N4	111.4 (8)	C19—C20—H20C	109.5
N3—C6—H6A	124.3	H20A—C20—H20C	109.5
N4—C6—H6A	124.3	H20B—C20—H20C	109.5
C8—C7—N4	105.8 (7)		

N3—Cu1—N1—C1	−51.1 (9)	C2—N2—C4—C5	74.7 (17)
N7—Cu1—N1—C1	134.5 (9)	C8—N3—C6—N4	−0.7 (11)
Cl1—Cu1—N1—C1	43.2 (8)	Cu1—N3—C6—N4	−171.2 (6)
N3—Cu1—N1—C3	134.9 (8)	C7—N4—C6—N3	0.7 (11)
N7—Cu1—N1—C3	−39.5 (8)	C9—N4—C6—N3	178.8 (8)
Cl1—Cu1—N1—C3	−130.8 (8)	C6—N4—C7—C8	−0.3 (10)
N1—Cu1—N3—C6	−90.4 (8)	C9—N4—C7—C8	−178.4 (8)
N5—Cu1—N3—C6	84.6 (8)	N4—C7—C8—N3	−0.1 (10)
Cl1—Cu1—N3—C6	176.9 (7)	C6—N3—C8—C7	0.5 (11)
N1—Cu1—N3—C8	101.2 (8)	Cu1—N3—C8—C7	170.7 (6)
N5—Cu1—N3—C8	−83.8 (8)	C6—N4—C9—C10	83.2 (14)
Cl1—Cu1—N3—C8	8.5 (8)	C7—N4—C9—C10	−99.0 (13)
N3—Cu1—N5—C11	−55.9 (9)	C13—N5—C11—N6	−0.7 (12)
N7—Cu1—N5—C11	118.7 (9)	Cu1—N5—C11—N6	−173.1 (7)
Cl1—Cu1—N5—C11	−150.1 (9)	C12—N6—C11—N5	1.4 (13)
N3—Cu1—N5—C13	133.0 (8)	C14—N6—C11—N5	178.2 (10)
N7—Cu1—N5—C13	−52.4 (8)	C11—N6—C12—C13	−1.4 (12)
Cl1—Cu1—N5—C13	38.8 (8)	C14—N6—C12—C13	−178.3 (10)
N1—Cu1—N7—C16	131.7 (8)	N6—C12—C13—N5	1.0 (12)
N5—Cu1—N7—C16	−43.6 (8)	C11—N5—C13—C12	−0.2 (12)
Cl1—Cu1—N7—C16	−135.8 (8)	Cu1—N5—C13—C12	172.6 (7)
N1—Cu1—N7—C18	−53.5 (8)	C11—N6—C14—C15	−74 (2)
N5—Cu1—N7—C18	131.2 (8)	C12—N6—C14—C15	102.6 (18)
Cl1—Cu1—N7—C18	39.0 (8)	C18—N7—C16—N8	−0.7 (11)
C3—N1—C1—N2	−1.2 (12)	Cu1—N7—C16—N8	174.9 (6)
Cu1—N1—C1—N2	−176.4 (7)	C17—N8—C16—N7	0.3 (11)
C2—N2—C1—N1	2.2 (13)	C19—N8—C16—N7	−177.5 (8)
C4—N2—C1—N1	178.0 (10)	C16—N8—C17—C18	0.2 (11)
C1—N2—C2—C3	−2.2 (12)	C19—N8—C17—C18	178.2 (9)

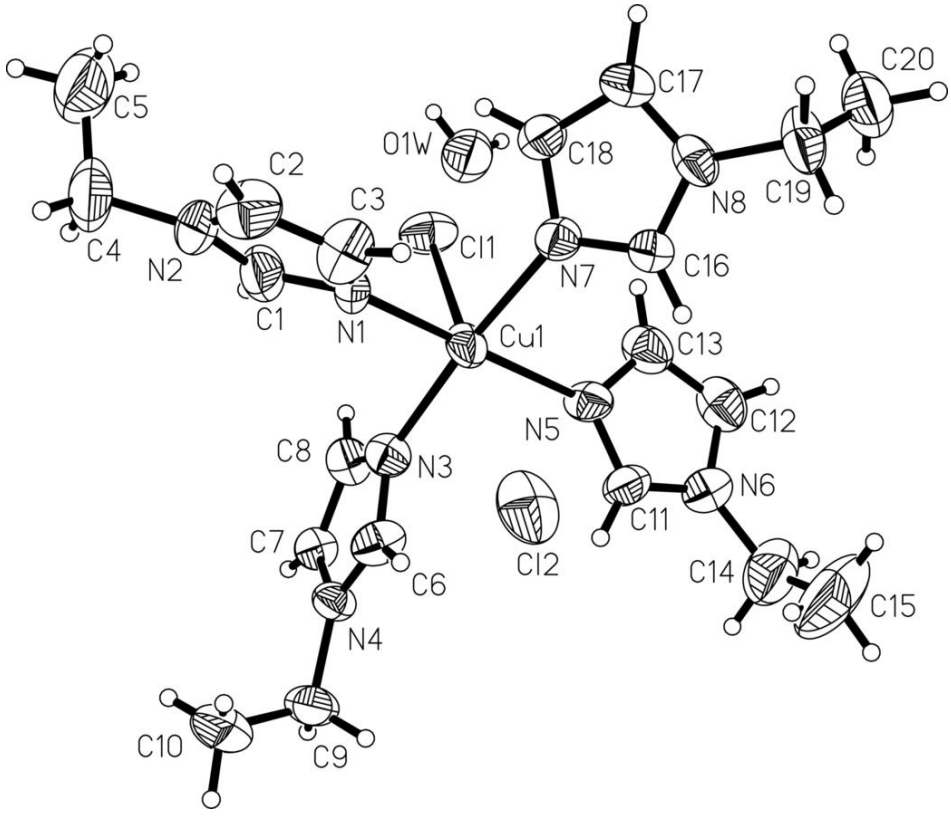
C4—N2—C2—C3	−178.0 (11)	C16—N7—C18—C17	0.9 (11)
N2—C2—C3—N1	1.6 (13)	Cu1—N7—C18—C17	−174.8 (6)
C1—N1—C3—C2	−0.3 (12)	N8—C17—C18—N7	−0.7 (11)
Cu1—N1—C3—C2	174.7 (8)	C16—N8—C19—C20	105.1 (12)
C1—N2—C4—C5	−100.3 (16)	C17—N8—C19—C20	−72.4 (13)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1WA···Cl2^{i}	0.84 (10)	2.47 (11)	3.206 (11)	147
O1W—H1WB···Cl1	0.85 (10)	2.39 (9)	3.183 (9)	156 (9)
C6—H6A···Cl2	0.93	2.61	3.401 (5)	143
C7—H7A···Cl2^{ii}	0.93	2.81	3.595 (6)	143
C9—H9B···Cl1^{iii}	0.97	2.72	3.598 (9)	151
C11—H11A···O1W^{iii}	0.93	2.47	3.361 (9)	161
C19—H19B···Cl1^{iv}	0.97	2.77	3.713 (12)	162

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

Fig. 1


C5
C2
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C16
C13
C12
N5
C8
N3
N6
C11
C7
Cl2
C6
C14
C15
N4
C10
C9

Fig. 2