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Tetrakis(1*H*-imidazole-κN^3)(perchlorato-κO)copper(II) perchlorate dimethylamine disolvate

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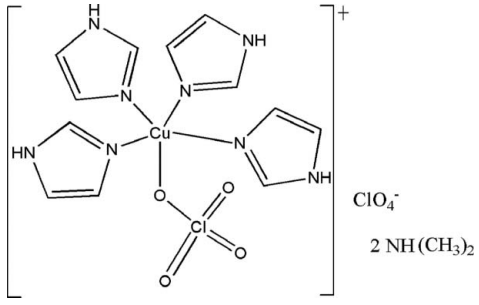
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.004 Å; R factor = 0.039; wR factor = 0.119; data-to-parameter ratio = 19.0.

The asymmetric unit of the title compound, $[Cu(ClO_4)(C_3H_4N_2)_4]ClO_4{\cdot}2C_2H_7N_2$, consists of a cationic tetrakis(1*H*-imidazole)perchloratocopper(II) complex, two dimethylamine solvent molecules and one perchlorate counter-anion. The coordination geometry of the metal atom is tetragonal-pyramidal, with four imidazole molecules in the basal plane and a perchlorate anion at the apex. The complex cations act as multiple connectors and self-assemble into a one-dimensional hydrogen-bonded ribbon, which is further hydrogen bonded with the perchlorate anion and solvent dimethylamine to form a two-dimensional framework.

Related literature

For related literature, see: Głowiak & Wnęk (1985); Lavalette *et al.* (2003); Moulton & Zaworotko (2001); Sengupta *et al.* (2001); Xu *et al.* (2004).



Experimental

Crystal data

$[Cu(ClO_4)(C_3H_4N_2)_4]ClO_4{\cdot}2C_2H_7N_2$
M_r = 624.94
Monoclinic, $P2_1/c$
a = 16.5302 (17) Å
b = 9.2777 (10) Å
c = 20.7248 (15) Å
β = 125.580 (5)°
V = 2585.0 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.11 mm^{-1}
T = 273 (2) K
0.32 × 0.29 × 0.25 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.712, T_{max} = 0.765
21182 measured reflections
6240 independent reflections
4989 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.119
S = 1.07
6240 reflections
328 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.66 e Å^{-3}
$\Delta\rho_{min}$ = −0.87 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N3	2.0104 (19)	Cu1—N7	2.0347 (19)
Cu1—N5	2.0151 (19)	Cu1—O1	2.2796 (19)
Cu1—N1	2.0223 (19)		
N3—Cu1—N5	90.64 (8)	N1—Cu1—N7	91.59 (8)
N3—Cu1—N1	87.23 (8)	N3—Cu1—O1	94.99 (8)
N5—Cu1—N1	162.13 (9)	N5—Cu1—O1	87.62 (7)
N3—Cu1—N7	172.14 (8)	N1—Cu1—O1	110.24 (8)
N5—Cu1—N7	88.11 (8)	N7—Cu1—O1	92.71 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···O4^{i}	0.88	2.21	3.013 (3)	152
N4—H4B···O4^{ii}	0.88	1.94	2.808 (3)	167
N8—H8B···O8^{iii}	0.88	1.95	2.828 (3)	177
N9—H9B···O5^{iii}	0.88	2.19	2.693 (3)	116
N9—H9B···O6^{iv}	0.88	2.33	2.717 (3)	107
N6—H6B···O6	0.88	2.11	2.924 (3)	154
N6—H6B···O8	0.88	2.27	3.001 (3)	140
N10—H10B···O3	0.90	2.13	2.749 (2)	126

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

Data collection: *SMART* (Siemens, 1994); cell refinement: *SAINT* (Siemens, 1994); data reduction: *SHELXTL* (Sheldrick, 1997*b*); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); 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: AT2354).

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supplementary materials

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Tetrakis(1*H*-imidazole-κN^3)(perchlorato-κO)copper(II) perchlorate dimethylamine disolvate

Y.-X. Zhou, G.-X. Cheng, B.-L. Wu and H.-Y. Zhang

Comment

In decades, hydrogen bonding with directionality and strength has been widely exploited by crystal engineers to control and tune structure topologies. For example, the carboxylic acid moiety as a graceful supramolecular synthon can be hydrogen bonded into not only discrete aggregates and one-dimensional polymers but also two-dimensional and three-dimensional networks; and calix-*C*-methylresorcin-[4]arenes self-assembled with water molecules held together by hydrogen bonds into a spheroid with a very large enclosed cavity of 1375 $Å^3$ (Moulton & Zaworotko, 2001). Of currently attractive are coordination complexes encoding multiple hydrogen-bonding acceptors and donors embedded in ligands because these supramolecular synthons incorporating stereostructure and H-bond sites can further construct higher-ordered aggregates through H-bond recognitions (Lavalette *et al.*, 2003; Głowiak & Wnęk, 1985). We communicate herein the synthesis and hydrogen-bonded two-dimensional planar sheet constructed by novel one-dimensional hydrogen-bonded ribbons of the title compound, $[Cu(C_3H_4N_2)_4(ClO_4)]^+\cdot(ClO_4)^-\cdot 2(C_2H_7N)$, (I).

In (I), the coordination enviroment of Cu(II) ion is axially elongated tetragonal-pyramidal (Fig. 1 and Table 1). The Cu(II) atom is Penta-coordinated by N_4O with four terminal imidazole molecules arranged almost perpendicular to the $Cu—N_4$ plane in base [Cu—N, from 2.0104 (19) to 2.0347 (19) Å] and a terminal perchlorate anion at apex [Cu—O, 2.2796 (19) Å]. As clearly shown in Fig. 2, the cation complex is an excellent supramolecular synthon. The four terminal imidazole ligands acting as hydrogen-bonding donors bind two lattice perchlorates and two coordination perchlorates, respectively, while, with the free coordination oxygen O4 as hydrogen-bonding acceptors, the coordination perchlorate anion also connect with two imidazole ligands from different complex ions (Table 2). Thus, the cation complex is a notable six-connector, and self-assembles into a novel one-dimensional hydrogen-bonded ribbon by paired N—H···O hydrogen bonds. With lattice perchlorate being captured at one corner by other paired N—H···O hydrogen bonds, the novel one-dimensional hydrogen-bonded ribbons finally extend into a hydrogen-bonded two-dimensional planar sheet in the direction parallel to the $(\bar{1}\ 0\ 1)$ plane (Fig. 3), and pack up in crystals (Fig. 4). Remarkably, through H-bond interactions, dimethylamine molecules which have been determined by single-crystal and elemental analysis inhabit in cavities of the one-dimensional hydrogen-bonded ribbons or ride at the lattice perchlorate. Perhaps, the dimethylamine derived from the decomposition of *N*,*N*-dimethylformamide in the reaction system (Xu *et al.*, 2004).

Experimental

A solution of imidazole (0.0272 g, 0.4 mmol) and *N*,*N*-dimethylformamide (5 ml) was mixed with a solution of $Cu(ClO_4)_2\cdot 6H_2O$ (0.0371 g, 0.1 mmol) in methanol (15 ml) with sharp stir. Then the mixture was heated for half an hour in water bath at 333 K, which led to a green solution. With the solution slowly evaporating in room temperature for three week, green block crystal appeared. Filtrated, washed with a few drops of methanol and dried naturally, pure title compound of 0.047 g was obtained (yield 75%); Analysis calculated for $C_{16}H_{30}Cl_2CuN_{10}O_8$: C 30.75, H 4.84, N 22.41%. Found: C 30.82, H 4.79, N 22.45%.

Refinement

All H atoms were positioned geometrically and constrained to ride on their parent atoms with C—H = 0.95–0.98 Å, N—H = 0.88–0.90 Å and with U_{iso} = 1.2U_{eq}(C, N) or 1.5U_{eq}(C) for methyl H atoms.

Figures

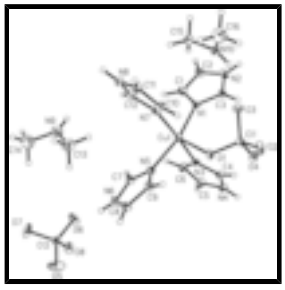

Fig. 1. An *ORTEP* representation of the asymmetry unit in the title compound (I), showing tetragonal-pyramidal coordination geometry around metal center Cu(II). Displacement ellipsoids are drawn at the 30% probability level.

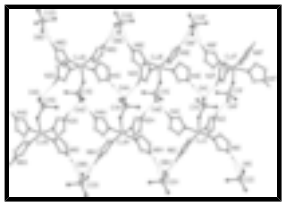

Fig. 2. View of the self-assembly of complex (I) into a novel one-dimensional hydrogen-bonded ribbon by paired N—H···O hydrogen bonds.

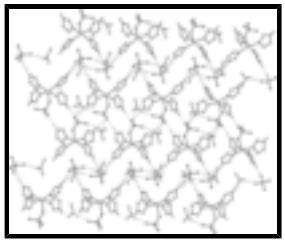

Fig. 3. View of a hydrogen-bonded two-dimensional planar sheet extending in the direction parallel to the ($\bar{1}$ 0 1) plane.

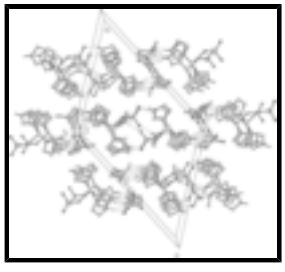

Fig. 4. Packing diagram of the title compound (I), showing guest dimethylamine molecules inhabited in the cavities (partial hydrogen atoms have been omitted for clarity).

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Crystal data

$[Cu(ClO_4)(C_3H_4N_2)_4]ClO_4{\cdot}2C_2H_7N_2$	F_{000} = 1292
M_r = 624.94	D_x = 1.606 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 6261 reflections

a = 16.5302 (17) Å	θ = 2.5–27.9º
b = 9.2777 (10) Å	μ = 1.11 mm^{-1}
c = 20.7248 (15) Å	T = 273 (2) K
β = 125.580 (5)º	Block, green
V = 2585.0 (5) Å^3	0.32 × 0.29 × 0.25 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	6240 independent reflections
Radiation source: fine-focus sealed tube	4989 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.030
T = 273(2) K	θ_{max} = 28.3º
φ and ω scans	θ_{min} = 2.4º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −22→21
T_{min} = 0.712, T_{max} = 0.765	k = −12→12
21182 measured reflections	l = −27→26

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.039	H-atom parameters constrained
$wR(F^2)$ = 0.119	$w = 1/[\sigma^2(F_o^2) + (0.0615P)^2 + 1.869P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max}$ = 0.001
6240 reflections	$\Delta\rho_{max}$ = 0.66 e Å^{-3}
328 parameters	$\Delta\rho_{min}$ = −0.87 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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	0.28355 (2)	0.24588 (3)	0.777041 (17)	0.02098 (10)
Cl1	0.52647 (4)	0.21986 (6)	0.92904 (3)	0.02249 (13)
O1	0.45053 (13)	0.28852 (19)	0.85304 (10)	0.0293 (4)
N1	0.25032 (16)	0.0965 (2)	0.82932 (12)	0.0243 (4)
C1	0.1562 (2)	0.0424 (3)	0.79480 (16)	0.0311 (5)
H1A	0.0997	0.0647	0.7429	0.037*
Cl2	0.04412 (4)	0.77614 (6)	0.43718 (3)	0.02472 (14)
O2	0.51351 (15)	0.2707 (2)	0.99015 (11)	0.0388 (5)
N2	0.25177 (17)	−0.0490 (2)	0.91358 (13)	0.0311 (5)
H2B	0.2736	−0.0988	0.9570	0.037*
C2	0.1568 (2)	−0.0483 (3)	0.84686 (16)	0.0318 (6)
H2C	0.1019	−0.1006	0.8382	0.038*
O3	0.51743 (15)	0.06216 (19)	0.92169 (12)	0.0402 (5)
N3	0.25347 (16)	0.3963 (2)	0.83014 (12)	0.0244 (4)
C3	0.30678 (19)	0.0401 (3)	0.90176 (15)	0.0269 (5)
H3B	0.3756	0.0595	0.9396	0.032*
O4	0.62696 (14)	0.26129 (18)	0.95327 (11)	0.0283 (4)
N4	0.26774 (17)	0.5529 (2)	0.91551 (13)	0.0311 (5)
H4B	0.2947	0.6063	0.9584	0.037*
C4	0.3164 (2)	0.4596 (3)	0.89952 (15)	0.0273 (5)
H4C	0.3859	0.4417	0.9332	0.033*
O5	0.01465 (19)	0.9259 (2)	0.43397 (19)	0.0682 (8)
N5	0.27036 (15)	0.3940 (2)	0.70031 (11)	0.0225 (4)
C5	0.1696 (2)	0.5503 (3)	0.85361 (16)	0.0343 (6)
H5B	0.1176	0.6056	0.8482	0.041*
O6	0.01920 (16)	0.6908 (3)	0.48374 (13)	0.0492 (6)
N6	0.2068 (2)	0.5493 (2)	0.60361 (13)	0.0435 (6)
H6B	0.1627	0.6045	0.5638	0.052*
C6	0.1612 (2)	0.4522 (3)	0.80090 (16)	0.0321 (6)
H6C	0.1010	0.4266	0.7518	0.039*
O7	−0.00792 (18)	0.7188 (3)	0.35769 (13)	0.0571 (7)
N7	0.29348 (15)	0.0923 (2)	0.71186 (12)	0.0235 (4)
C7	0.1884 (2)	0.4609 (3)	0.64449 (15)	0.0326 (6)
H7B	0.1251	0.4481	0.6347	0.039*
O8	0.15263 (14)	0.7693 (2)	0.47831 (12)	0.0352 (4)
N8	0.25757 (17)	−0.0565 (2)	0.61590 (12)	0.0316 (5)
H8B	0.2230	−0.1104	0.5731	0.038*
C8	0.3048 (3)	0.5398 (3)	0.63370 (17)	0.0425 (7)
H8C	0.3388	0.5906	0.6164	0.051*
C9	0.3441 (2)	0.4422 (3)	0.69392 (16)	0.0309 (5)
H9A	0.4117	0.4123	0.7263	0.037*
C10	0.38020 (19)	0.0519 (3)	0.72164 (15)	0.0282 (5)
H10A	0.4451	0.0835	0.7631	0.034*
C11	0.3582 (2)	−0.0407 (3)	0.66236 (16)	0.0311 (5)
H11A	0.4040	−0.0853	0.6550	0.037*

C12	0.21965 (11)	0.02468 (15)	0.64659 (9)	0.0289 (5)
H12A	0.1510	0.0325	0.6251	0.035*
N10	0.42910 (11)	−0.20296 (15)	0.86560 (9)	0.0321 (5)
H10B	0.4422	−0.1364	0.9021	0.038*
N9	0.06492 (11)	0.20562 (15)	0.44547 (9)	0.0434 (6)
H9B	0.0467	0.1522	0.4701	0.052*
C13	0.1675 (3)	0.2473 (4)	0.4811 (3)	0.0596 (10)
H13A	0.2102	0.2075	0.5348	0.089*
H13B	0.1727	0.3526	0.4835	0.089*
H13C	0.1886	0.2098	0.4488	0.089*
C14	−0.0058 (4)	0.2612 (4)	0.3643 (3)	0.0669 (11)
H14A	−0.0733	0.2299	0.3441	0.100*
H14B	0.0120	0.2239	0.3298	0.100*
H14C	−0.0031	0.3668	0.3650	0.100*
C15	0.3270 (3)	−0.2450 (3)	0.79940 (18)	0.0380 (7)
H15A	0.2788	−0.1894	0.8023	0.057*
H15B	0.3174	−0.3481	0.8032	0.057*
H15C	0.3171	−0.2255	0.7488	0.057*
C16	0.5070 (3)	−0.2820 (4)	0.8665 (2)	0.0578 (9)
H16A	0.5726	−0.2499	0.9117	0.087*
H16B	0.5004	−0.2632	0.8171	0.087*
H16C	0.4997	−0.3856	0.8712	0.087*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.03030 (18)	0.01577 (14)	0.02325 (16)	0.00019 (11)	0.01922 (14)	0.00038 (10)
Cl1	0.0205 (3)	0.0258 (3)	0.0189 (3)	−0.0009 (2)	0.0102 (2)	0.0005 (2)
O1	0.0261 (10)	0.0329 (9)	0.0209 (8)	0.0013 (7)	0.0091 (8)	0.0040 (7)
N1	0.0319 (11)	0.0206 (9)	0.0251 (10)	−0.0007 (8)	0.0191 (9)	0.0013 (8)
C1	0.0279 (14)	0.0321 (13)	0.0299 (13)	0.0001 (10)	0.0148 (11)	0.0064 (11)
Cl2	0.0223 (3)	0.0272 (3)	0.0228 (3)	−0.0005 (2)	0.0120 (2)	0.0007 (2)
O2	0.0337 (11)	0.0634 (14)	0.0236 (9)	0.0114 (9)	0.0192 (9)	0.0030 (8)
N2	0.0388 (13)	0.0302 (11)	0.0302 (11)	0.0049 (9)	0.0234 (10)	0.0096 (9)
C2	0.0299 (14)	0.0314 (13)	0.0374 (14)	−0.0029 (11)	0.0216 (12)	0.0051 (11)
O3	0.0384 (12)	0.0222 (9)	0.0433 (11)	−0.0062 (8)	0.0143 (10)	0.0013 (8)
N3	0.0310 (11)	0.0200 (9)	0.0267 (10)	−0.0010 (8)	0.0194 (9)	−0.0029 (8)
C3	0.0291 (13)	0.0264 (12)	0.0272 (12)	−0.0006 (10)	0.0176 (11)	0.0005 (10)
O4	0.0224 (9)	0.0373 (10)	0.0257 (9)	−0.0079 (7)	0.0143 (8)	−0.0061 (7)
N4	0.0393 (13)	0.0277 (11)	0.0267 (10)	−0.0026 (9)	0.0193 (10)	−0.0092 (9)
C4	0.0301 (13)	0.0245 (11)	0.0268 (12)	−0.0008 (10)	0.0162 (11)	−0.0017 (9)
O5	0.0570 (16)	0.0278 (11)	0.129 (2)	0.0085 (10)	0.0591 (18)	0.0038 (13)
N5	0.0247 (11)	0.0199 (9)	0.0231 (9)	0.0013 (8)	0.0140 (9)	0.0025 (7)
C5	0.0332 (15)	0.0359 (14)	0.0361 (14)	0.0015 (11)	0.0215 (13)	−0.0085 (12)
O6	0.0421 (13)	0.0645 (14)	0.0445 (12)	−0.0002 (11)	0.0272 (11)	0.0217 (11)
N6	0.0555 (17)	0.0292 (12)	0.0263 (11)	0.0066 (11)	0.0126 (12)	0.0112 (9)
C6	0.0294 (14)	0.0361 (14)	0.0311 (13)	−0.0024 (11)	0.0178 (12)	−0.0101 (11)
O7	0.0407 (14)	0.0908 (19)	0.0264 (11)	−0.0196 (12)	0.0119 (10)	−0.0220 (11)

N7	0.0296 (11)	0.0200 (9)	0.0246 (10)	0.0004 (8)	0.0178 (9)	−0.0011 (8)
C7	0.0286 (14)	0.0286 (12)	0.0291 (13)	0.0034 (10)	0.0102 (11)	0.0003 (10)
O8	0.0199 (10)	0.0517 (12)	0.0274 (9)	0.0010 (8)	0.0099 (8)	0.0011 (8)
N8	0.0403 (13)	0.0263 (11)	0.0245 (10)	−0.0054 (9)	0.0168 (10)	−0.0074 (8)
C8	0.064 (2)	0.0360 (15)	0.0364 (15)	−0.0126 (14)	0.0343 (16)	0.0014 (12)
C9	0.0320 (14)	0.0340 (13)	0.0323 (13)	−0.0027 (11)	0.0219 (12)	0.0036 (11)
C10	0.0285 (13)	0.0300 (12)	0.0281 (12)	−0.0045 (10)	0.0177 (11)	−0.0077 (10)
C11	0.0334 (14)	0.0318 (13)	0.0319 (13)	0.0001 (11)	0.0212 (12)	−0.0067 (11)
C12	0.0304 (14)	0.0259 (12)	0.0280 (12)	−0.0013 (10)	0.0157 (11)	−0.0009 (10)
N10	0.0443 (14)	0.0265 (10)	0.0293 (11)	−0.0029 (10)	0.0237 (11)	−0.0048 (9)
N9	0.0523 (17)	0.0352 (12)	0.0491 (15)	−0.0021 (12)	0.0331 (14)	0.0038 (11)
C13	0.064 (3)	0.054 (2)	0.064 (3)	−0.0127 (17)	0.040 (2)	−0.0039 (17)
C14	0.073 (3)	0.071 (3)	0.057 (2)	0.008 (2)	0.037 (2)	0.0065 (18)
C15	0.0472 (19)	0.0309 (14)	0.0317 (14)	−0.0038 (12)	0.0206 (14)	−0.0025 (11)
C16	0.061 (2)	0.064 (2)	0.064 (2)	0.0081 (18)	0.045 (2)	−0.0023 (18)

Geometric parameters (Å, °)

Cu1—N3	2.0104 (19)	N6—H6B	0.8800
Cu1—N5	2.0151 (19)	C6—H6C	0.9500
Cu1—N1	2.0223 (19)	N7—C12	1.339 (2)
Cu1—N7	2.0347 (19)	N7—C10	1.378 (3)
Cu1—O1	2.2796 (19)	C7—H7B	0.9500
Cl1—O3	1.4695 (19)	N8—C12	1.352 (3)
Cl1—O1	1.4702 (18)	N8—C11	1.361 (4)
Cl1—O2	1.4794 (19)	N8—H8B	0.8800
Cl1—O4	1.4794 (18)	C8—C9	1.362 (4)
N1—C3	1.330 (3)	C8—H8C	0.9500
N1—C1	1.375 (3)	C9—H9A	0.9500
C1—C2	1.363 (3)	C10—C11	1.363 (3)
C1—H1A	0.9500	C10—H10A	0.9500
Cl2—O7	1.445 (2)	C11—H11A	0.9500
Cl2—O5	1.461 (2)	C12—H12A	0.9500
Cl2—O8	1.473 (2)	N10—C16	1.472 (4)
Cl2—O6	1.480 (2)	N10—C15	1.480 (4)
N2—C3	1.352 (3)	N10—H10B	0.9000
N2—C2	1.360 (4)	N9—C13	1.454 (4)
N2—H2B	0.8800	N9—C14	1.475 (4)
C2—H2C	0.9500	N9—H9B	0.8800
N3—C4	1.324 (3)	C13—H13A	0.9800
N3—C6	1.374 (3)	C13—H13B	0.9800
C3—H3B	0.9500	C13—H13C	0.9800
N4—C4	1.348 (3)	C14—H14A	0.9800
N4—C5	1.362 (4)	C14—H14B	0.9800
N4—H4B	0.8800	C14—H14C	0.9800
C4—H4C	0.9500	C15—H15A	0.9800
N5—C7	1.317 (3)	C15—H15B	0.9800
N5—C9	1.375 (3)	C15—H15C	0.9800
C5—C6	1.365 (3)	C16—H16A	0.9800

C5—H5B	0.9500	C16—H16B	0.9800
N6—C7	1.335 (4)	C16—H16C	0.9800
N6—C8	1.359 (4)		
N3—Cu1—N5	90.64 (8)	C5—C6—H6C	125.4
N3—Cu1—N1	87.23 (8)	N3—C6—H6C	125.4
N5—Cu1—N1	162.13 (9)	C12—N7—C10	106.26 (17)
N3—Cu1—N7	172.14 (8)	C12—N7—Cu1	128.37 (14)
N5—Cu1—N7	88.11 (8)	C10—N7—Cu1	124.88 (16)
N1—Cu1—N7	91.59 (8)	N5—C7—N6	110.4 (2)
N3—Cu1—O1	94.99 (8)	N5—C7—H7B	124.8
N5—Cu1—O1	87.62 (7)	N6—C7—H7B	124.8
N1—Cu1—O1	110.24 (8)	C12—N8—C11	108.51 (19)
N7—Cu1—O1	92.71 (7)	C12—N8—H8B	125.7
O3—Cl1—O1	110.39 (11)	C11—N8—H8B	125.7
O3—Cl1—O2	110.46 (12)	N6—C8—C9	105.6 (2)
O1—Cl1—O2	108.68 (11)	N6—C8—H8C	127.2
O3—Cl1—O4	108.68 (11)	C9—C8—H8C	127.2
O1—Cl1—O4	109.96 (11)	C8—C9—N5	109.1 (3)
O2—Cl1—O4	108.65 (11)	C8—C9—H9A	125.4
Cl1—O1—Cu1	126.93 (11)	N5—C9—H9A	125.4
C3—N1—C1	106.4 (2)	C11—C10—N7	109.2 (2)
C3—N1—Cu1	130.05 (18)	C11—C10—H10A	125.4
C1—N1—Cu1	123.33 (16)	N7—C10—H10A	125.4
C2—C1—N1	109.2 (2)	N8—C11—C10	106.3 (2)
C2—C1—H1A	125.4	N8—C11—H11A	126.8
N1—C1—H1A	125.4	C10—C11—H11A	126.8
O7—Cl2—O5	109.68 (17)	N7—C12—N8	109.67 (16)
O7—Cl2—O8	111.14 (13)	N7—C12—H12A	125.2
O5—Cl2—O8	109.20 (13)	N8—C12—H12A	125.2
O7—Cl2—O6	109.84 (15)	C16—N10—C15	113.4 (2)
O5—Cl2—O6	109.05 (15)	C16—N10—H10B	123.4
O8—Cl2—O6	107.88 (12)	C15—N10—H10B	123.2
C3—N2—C2	108.2 (2)	C13—N9—C14	113.7 (3)
C3—N2—H2B	125.9	C13—N9—H9B	123.1
C2—N2—H2B	125.9	C14—N9—H9B	123.1
N2—C2—C1	106.3 (2)	N9—C13—H13A	109.5
N2—C2—H2C	126.9	N9—C13—H13B	109.5
C1—C2—H2C	126.9	H13A—C13—H13B	109.5
C4—N3—C6	106.3 (2)	N9—C13—H13C	109.5
C4—N3—Cu1	127.88 (17)	H13A—C13—H13C	109.5
C6—N3—Cu1	125.83 (17)	H13B—C13—H13C	109.5
N1—C3—N2	109.9 (2)	N9—C14—H14A	109.5
N1—C3—H3B	125.0	N9—C14—H14B	109.5
N2—C3—H3B	125.0	H14A—C14—H14B	109.5
C4—N4—C5	108.1 (2)	N9—C14—H14C	109.5
C4—N4—H4B	125.9	H14A—C14—H14C	109.5
C5—N4—H4B	125.9	H14B—C14—H14C	109.5
N3—C4—N4	110.4 (2)	N10—C15—H15A	109.5
N3—C4—H4C	124.8	N10—C15—H15B	109.5

N4—C4—H4C	124.8	H15A—C15—H15B	109.5
C7—N5—C9	106.2 (2)	N10—C15—H15C	109.5
C7—N5—Cu1	126.73 (18)	H15A—C15—H15C	109.5
C9—N5—Cu1	127.08 (17)	H15B—C15—H15C	109.5
N4—C5—C6	106.1 (2)	N10—C16—H16A	109.5
N4—C5—H5B	127.0	N10—C16—H16B	109.5
C6—C5—H5B	127.0	H16A—C16—H16B	109.5
C7—N6—C8	108.7 (2)	N10—C16—H16C	109.5
C7—N6—H6B	125.7	H16A—C16—H16C	109.5
C8—N6—H6B	125.7	H16B—C16—H16C	109.5
C5—C6—N3	109.2 (2)		
O3—Cl1—O1—Cu1	51.84 (16)	N1—Cu1—N5—C7	15.6 (4)
O2—Cl1—O1—Cu1	−69.45 (16)	N7—Cu1—N5—C7	104.9 (2)
O4—Cl1—O1—Cu1	171.74 (11)	O1—Cu1—N5—C7	−162.3 (2)
N3—Cu1—O1—Cl1	89.35 (14)	N3—Cu1—N5—C9	114.8 (2)
N5—Cu1—O1—Cl1	179.78 (14)	N1—Cu1—N5—C9	−162.2 (2)
N1—Cu1—O1—Cl1	0.47 (16)	N7—Cu1—N5—C9	−72.9 (2)
N7—Cu1—O1—Cl1	−92.23 (14)	O1—Cu1—N5—C9	19.9 (2)
N3—Cu1—N1—C3	−84.1 (2)	C4—N4—C5—C6	0.5 (3)
N5—Cu1—N1—C3	−167.5 (2)	N4—C5—C6—N3	−0.5 (3)
N7—Cu1—N1—C3	103.7 (2)	C4—N3—C6—C5	0.2 (3)
O1—Cu1—N1—C3	10.3 (2)	Cu1—N3—C6—C5	179.30 (18)
N3—Cu1—N1—C1	89.9 (2)	N5—Cu1—N7—C12	−84.60 (17)
N5—Cu1—N1—C1	6.5 (4)	N1—Cu1—N7—C12	77.53 (18)
N7—Cu1—N1—C1	−82.3 (2)	O1—Cu1—N7—C12	−172.12 (17)
O1—Cu1—N1—C1	−175.75 (18)	N5—Cu1—N7—C10	86.23 (19)
C3—N1—C1—C2	−0.7 (3)	N1—Cu1—N7—C10	−111.65 (19)
Cu1—N1—C1—C2	−175.89 (17)	O1—Cu1—N7—C10	−1.30 (19)
C3—N2—C2—C1	0.2 (3)	C9—N5—C7—N6	−0.3 (3)
N1—C1—C2—N2	0.3 (3)	Cu1—N5—C7—N6	−178.51 (17)
N5—Cu1—N3—C4	−105.0 (2)	C8—N6—C7—N5	0.1 (3)
N1—Cu1—N3—C4	92.8 (2)	C7—N6—C8—C9	0.1 (3)
O1—Cu1—N3—C4	−17.3 (2)	N6—C8—C9—N5	−0.3 (3)
N5—Cu1—N3—C6	76.1 (2)	C7—N5—C9—C8	0.4 (3)
N1—Cu1—N3—C6	−86.1 (2)	Cu1—N5—C9—C8	178.57 (18)
O1—Cu1—N3—C6	163.8 (2)	C12—N7—C10—C11	−0.3 (3)
C1—N1—C3—N2	0.8 (3)	Cu1—N7—C10—C11	−172.86 (17)
Cu1—N1—C3—N2	175.60 (16)	C12—N8—C11—C10	−0.1 (3)
C2—N2—C3—N1	−0.7 (3)	N7—C10—C11—N8	0.3 (3)
C6—N3—C4—N4	0.1 (3)	C10—N7—C12—N8	0.3 (2)
Cu1—N3—C4—N4	−178.94 (16)	Cu1—N7—C12—N8	172.43 (15)
C5—N4—C4—N3	−0.4 (3)	C11—N8—C12—N7	−0.1 (2)
N3—Cu1—N5—C7	−67.3 (2)		

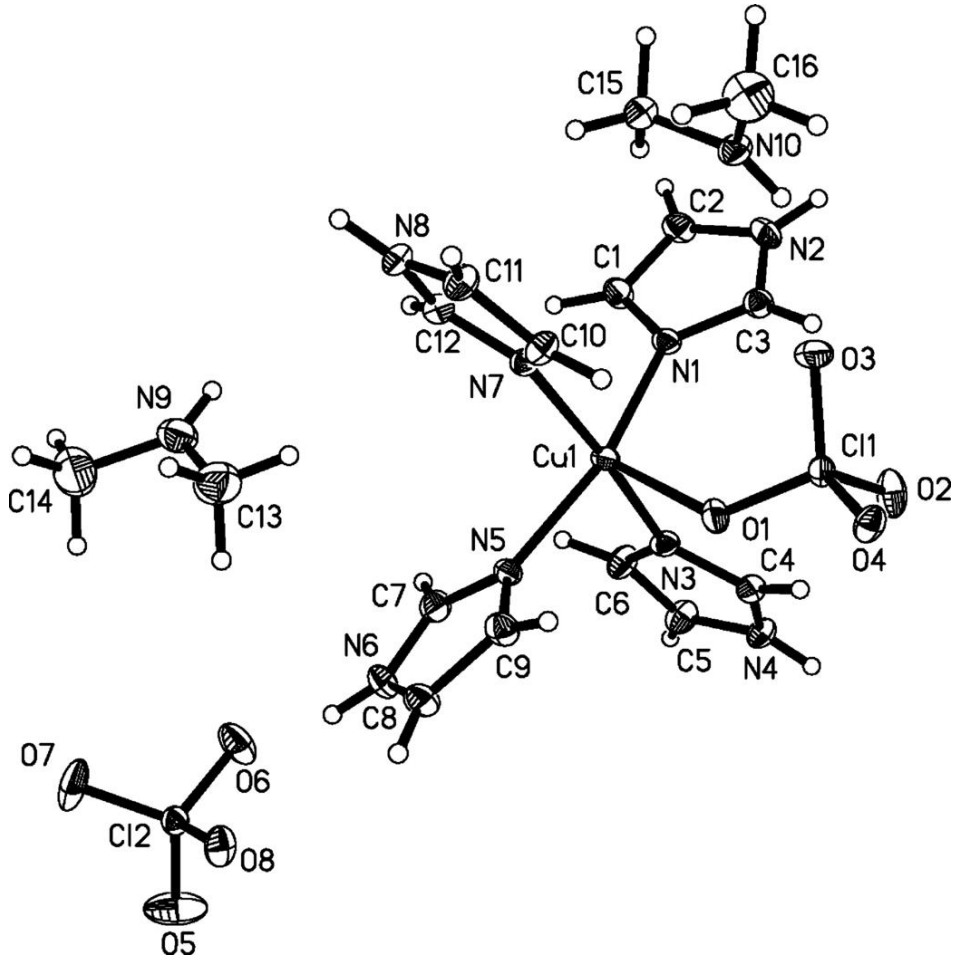
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2B···O4^{i}	0.88	2.21	3.013 (3)	152

N4—H4B···O4^{ii}	0.88	1.94	2.808 (3)	167
N8—H8B···O8^{iii}	0.88	1.95	2.828 (3)	177
N9—H9B···O5^{iii}	0.88	2.19	2.693 (3)	116
N9—H9B···O6^{iv}	0.88	2.33	2.717 (3)	107
N6—H6B···O6	0.88	2.11	2.924 (3)	154
N6—H6B···O8	0.88	2.27	3.001 (3)	140
N10—H10B···O3	0.90	2.13	2.749 (2)	126

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

Fig. 1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C2
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C10
C3
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N7
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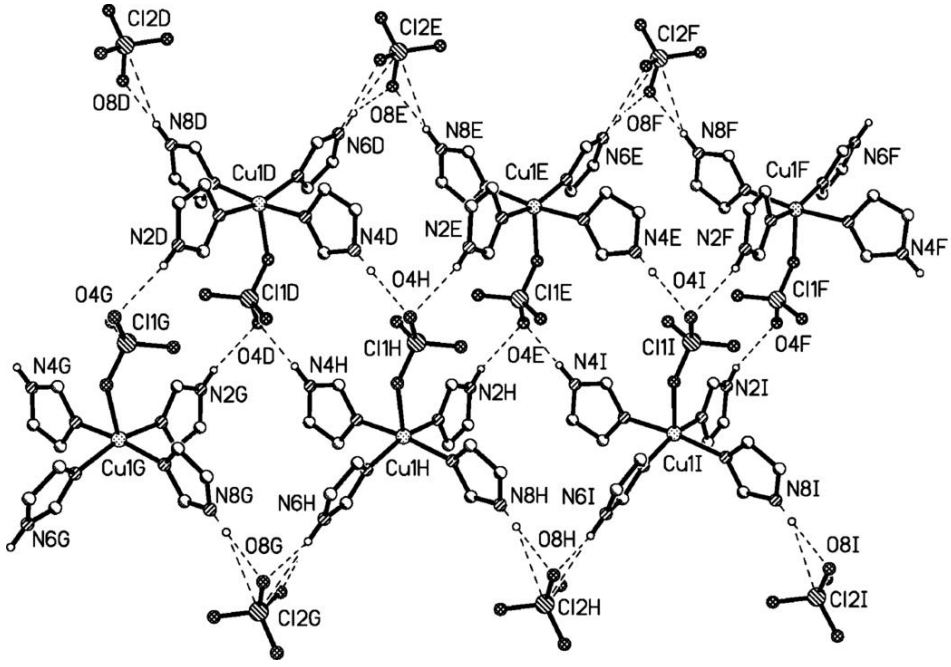
Cl1
O2
C14
C13
O1
N5
C4
O4
N3
C7
C6
N6
C9
C5
N4
C8
O7
O6
Cl2
O8
O5

Fig. 2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N8G
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Fig. 3

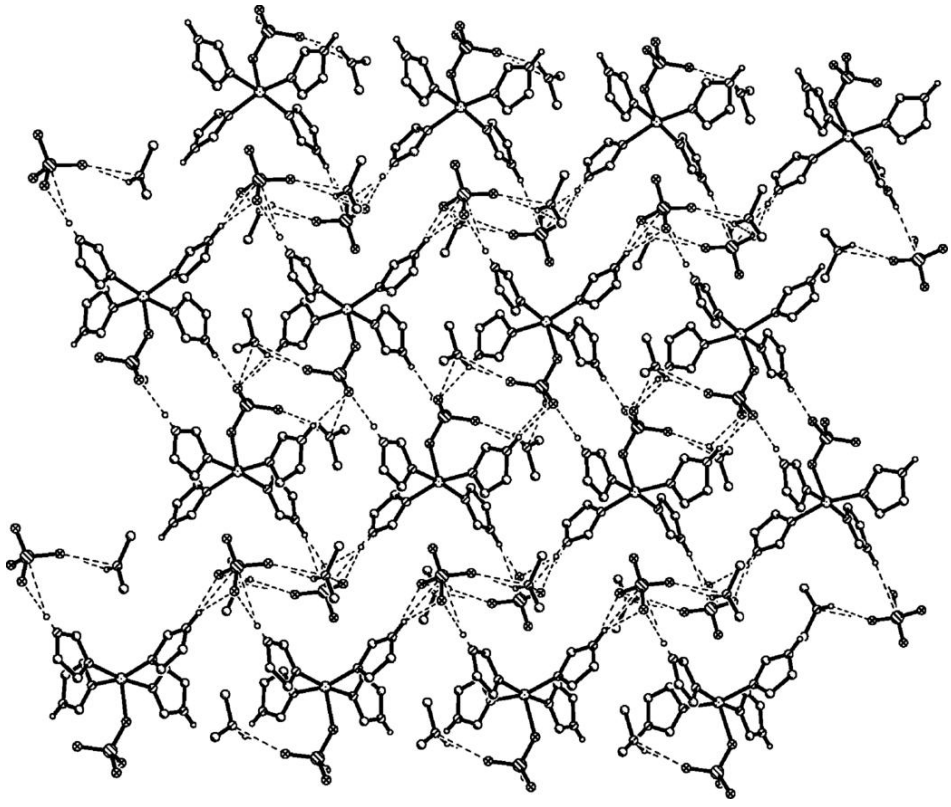

Fig. 4