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μ-Chlorido-bis({*N*-benzyl-*N*′-[2-(benzylamino)ethyl]ethane-1,2-diamine}chloridocopper(II)) chloride

Yu-Fen Liu,[a]* Hai-Tao Xia,[a] Da-Qi Wang[b] and Shu-Ping Yang[a]

[a]Department of Chemical Engineering, Huaihai Institute of Technology, Lianyungang, Jiangsu 222005, People's Republic of China, and [b]College of Chemistry and Chemical Engineering, Liaocheng University, Shandong 252059, People's Republic of China.
Correspondence e-mail: liu222005@hhit.edu.cn

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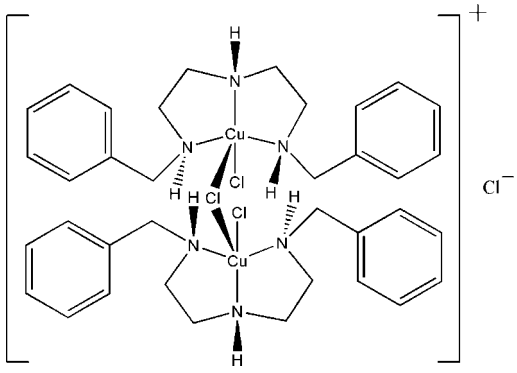
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.015 Å; R factor = 0.056; wR factor = 0.103; data-to-parameter ratio = 15.5.

In the title compound, $[Cu_2Cl_3(C_{18}H_{25}N_3)_2]Cl$, the asymmetric unit consists of one half of a μ-chlorido-bis[{*N*-benzyl-*N*′-[2-(benzylamino)ethyl]ethane-1,2-diamine}chloridocopper(II)] complex cation and one chloride anion lying on a twofold rotation axis. The two Cu^{II} centres are symmetry-related by a twofold rotation axis passing through the bridging Cl atom. The Cu atoms exhibit a distorted square-pyramidal coordination environment. The basal and apical Cu—Cl bond lengths are 2.254 (2) and 2.658 (2) Å, respectively. The Cu···Cu distance and Cu—Cl—Cu angle are 4.349 (6) Å and 109.8 (2)°, respectively. In the crystal structure, the molecules of the complex are linked into chains along *b* and *a* by C—H···π hydrogen bonds. The chloride anion links these chains along *c* into a three-dimensional network structure.

Related literature

For related literature, see: Lee *et al.* (2005); Rapheal *et al.* (2007).



Experimental

Crystal data

$[Cu_2Cl_3(C_{18}H_{25}N_3)_2]Cl$
M_r = 835.70
Monoclinic, $C2$
a = 25.584 (3) Å
b = 7.4506 (11) Å
c = 11.5739 (15) Å
β = 113.926 (2)°
V = 2016.6 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.35 mm^{-1}
T = 298 (2) K
0.27 × 0.14 × 0.11 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.712, T_{max} = 0.866
5224 measured reflections
3398 independent reflections
1758 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.103
S = 1.00
3398 reflections
219 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.91 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}
Absolute structure: Flack (1983), 1474 Friedel pairs
Flack parameter: 0.02 (3)

Table 1
Selected bond lengths (Å).

Cu1—N2	1.999 (7)	Cu1—Cl1	2.254 (2)
Cu1—N3	2.035 (6)	Cu1—Cl2	2.658 (2)
Cu1—N1	2.055 (6)		

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

*Cg*1 is the centroid of the C6–C11 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3*A*···Cl3	0.97	2.82	3.640 (11)	143
C2—H2*A*···*Cg*1^{i}	0.97	2.74	3.547 (9)	141
C15—H15···*Cg*1^{ii}	0.93	2.97	3.872 (14)	163

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); 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: BG2104).

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supplementary materials

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μ-Chlorido-bis({*N*-benzyl-*N*'-[2-(benzylamino)ethyl]ethane-1,2-diamine}chloridocopper(II)) chloride

Y.-F. Liu, H.-T. Xia, D.-Q. Wang and S.-P. Yang

Comment

Dinuclear copper(II) complexes, especially those containing a chlorine bridging ligand, have been the subject of extensive reseach because of their magnetic exchange interactions between ligand-bridged copper atoms, which mimic the biological active site in copper proteins (Lee *et al.*, 2005; Rapheal *et al.*, 2007). In the classical case, the copper atom is five coordinate and bridged by a monochlorine atom or eventually two chlorine atoms, depending on the coordination environment. Here, we report the synthesis and crystal structure of a new monochlorine bridged dicopper(II) complex, $[Cu_2\ Cl_3\ (C_{18}\ H_{25}\ N_3)_2]^+\cdot Cl^-$ (I).

In complex (I), the copper atom is five coordinated by one tridentate chelating (*N*-benzyl-*N*'-[2-(benzylamino)ethyl)]ethane-1,2-diamine) ligand and two chloride atoms, to form a distorted square pyramid geometry (Fig. 1). Three N atoms of the ligand and a monodentate chlorine are at the basal square plane, while the bridging chlorine atom is at the apical position. The Cu1 atom is shifted by 0.202 (3)Å from the basal plane towards the apical site. The dihedral angles between the basal plane and the C6—C11 (*Cg*1) and C13—C18 (*Cg*2) phenyl rings are 48.9 (3)° and 62.1 (3)°, respectively. Coordination distances are shown in Table 1. The Cu···Cu separation is 4.349 (6) Å, and the Cu—Cl—Cu angle is 109.8 (2)°.

In the crystal structure, C—H···π hydrogen bonds link the molecules into two types of chains running along *b* and *a* respectively (Fig. 2 and 3, Table 2). The chloride anion,, which also resides on a two fold axis, in turn, link these chains along the *c* direction (Fig. 4, Table 2), into a three-dimensinal network structure.

Experimental

N^1-benzyl-N^2-(2-(benzylamino)ethyl)ethane-1,2-diamine (4 mmol) was dissolved in ethanol (20 ml), and an aqueous solution (10 ml) of cupric chloride (2 mmol) was added. The reaction mixture was stirred 4 h at 323–333k. The solution was then cooled slowly to room temperature and filtered. Blue crystals suitable for X-ray diffraction were obtained by evaporation of an ethanol solution.

Refinement

The space group was uniquely assigned from the systematic absences. All H atoms were located in difference Fourier maps. H atoms bonded to C and N atoms were treated as riding atoms, with C—H distances of 0.93 Å (aryl), 0.97 Å(methylene) and N—H distances of 0.91 Å (amine), and with U_{iso}(H) = 1.2U_{eq}(C,*N*) (aryl, methylene, amine).

Figures

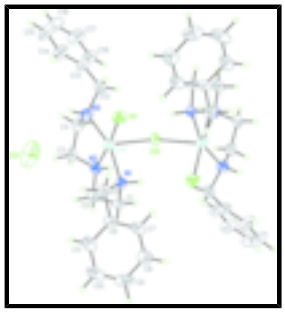

Fig. 1. The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids drawn at a 30% probability level. Unlabelled atoms in the cation are related to labelled ones by (−*x*, *y*, −*z*).

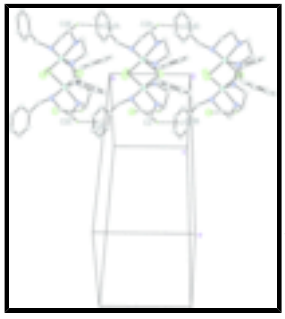

Fig. 2. A partial packing view of (I), showing the formation of a hydrogen-bonded chain along b, built from C—H···*Cg*1(π) interactions, *Cg*1: C6—C11. For clarity, H atoms not involved in hydrogen bonding have been omitted. Dashed lines indicate hydrogen bonds. [symmetry code: (A) − *x*, *y*, − *z*, (B) *x*, −1 + *y*, *z*, (C) *x*, 1 + *y*, − *z*, (D) − *x*, − 1 + *y*, − *z*, (E) − *x*, 1 + *y*, −*z*].

Fig. 3. A partial packing view of (I), showing the formation of a hydrogen-bonded chain along a, built from C—H···*Cg*1(π) interactions, *Cg*1: C6—C11. For clarity, H atoms not involved in hydrogen bonding have been omitted. Dashed lines indicate hydrogen bonds. [symmetry code: (A) − *x*, *y*, − *z*, (I) 1/2 − *x*, −1/2 + *y*, − *z*, (J) 1 − *x*, −1 + *y*, − *z*].

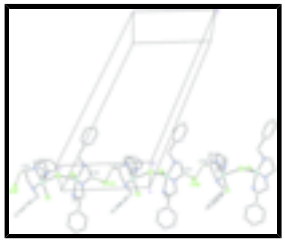

Fig. 4. A partial packing view of (I), showing the C—H···Cl interaction linking the above referenced chains along c. For clarity, H atoms not involved in the hydrogen bonding have been omitted. Dashed lines indicate hydrogen bonds. [symmetry code: (A) − *x*, *y*, − *z*, (F) *x*, *y*, 1 + *z*, (G) *x*, *y*, − 1 + *z*, (H) − *x*, *y*, 1 − *z*].

μ-Chlorido-bis({*N*-benzyl-*N*'-[2-(benzylamino)ethyl]ethane- 1,2-diamine}chloridocopper(II))

Crystal data

$[Cu_2Cl_3(C_{18}H_{25}N_3)_2]Cl$	F_{000} = 868
M_r = 835.70	D_x = 1.376 Mg m^{-3}
Monoclinic, *C*2	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: C 2y	Cell parameters from 896 reflections
a = 25.584 (3) Å	θ = 2.9–25.3°
b = 7.4506 (11) Å	μ = 1.35 mm^{-1}
c = 11.5739 (15) Å	*T* = 298 (2) K
β = 113.926 (2)°	Block, blue
V = 2016.6 (5) Å^3	0.27 × 0.14 × 0.11 mm
Z = 2	

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	3398 independent reflections
Radiation source: fine-focus sealed tube	1758 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.056$
$T = 298(2)$ K	$\theta_{max} = 25.0^{o}$
φ and ω scans	$\theta_{min} = 1.7^{o}$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -28 \rightarrow 30$
$T_{min} = 0.712$, $T_{max} = 0.866$	$k = -8 \rightarrow 8$
5224 measured reflections	$l = -12 \rightarrow 13$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.056$	$w = 1/[\sigma^2(F_o^2) + (0.0208P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.103$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.00$	$\Delta\rho_{max} = 0.91$ e Å^{-3}
3398 reflections	$\Delta\rho_{min} = -0.40$ e Å^{-3}
219 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), 1474 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.02 (3)
Secondary atom site location: difference Fourier map	

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	−0.00397 (4)	0.58358 (18)	0.18416 (10)	0.0507 (3)
Cl1	−0.06597 (8)	0.8020 (3)	0.0790 (2)	0.0635 (7)
Cl2	0.0000	0.3784 (4)	0.0000	0.0528 (9)

Cl3	0.0000	0.7398 (8)	0.5000	0.176 (3)
N1	0.0678 (2)	0.7293 (9)	0.2071 (6)	0.0408 (18)
H1	0.0658	0.7572	0.1288	0.049*
N2	0.0526 (3)	0.4103 (10)	0.3005 (6)	0.054 (2)
H2	0.0581	0.3252	0.2501	0.065*
N3	−0.0622 (3)	0.4348 (10)	0.2208 (7)	0.056 (2)
H3	−0.0721	0.5016	0.2746	0.067*
C1	0.1169 (3)	0.6147 (12)	0.2676 (8)	0.047 (2)
H1A	0.1509	0.6873	0.3088	0.057*
H1B	0.1225	0.5401	0.2048	0.057*
C2	0.1072 (3)	0.4948 (11)	0.3664 (8)	0.056 (3)
H2A	0.1372	0.4053	0.3995	0.067*
H2B	0.1070	0.5667	0.4360	0.067*
C3	0.0265 (4)	0.3159 (13)	0.3769 (8)	0.060 (3)
H3A	0.0276	0.3921	0.4457	0.072*
H3B	0.0476	0.2069	0.4125	0.072*
C4	−0.0348 (4)	0.2709 (13)	0.2912 (9)	0.062 (3)
H4A	−0.0357	0.1764	0.2327	0.074*
H4B	−0.0551	0.2293	0.3411	0.074*
C5	0.0710 (3)	0.8999 (12)	0.2756 (8)	0.057 (3)
H5A	0.0680	0.8734	0.3547	0.068*
H5B	0.0386	0.9743	0.2256	0.068*
C6	0.1253 (3)	1.0044 (10)	0.3033 (9)	0.048 (2)
C7	0.1353 (3)	1.0868 (16)	0.2091 (8)	0.060 (2)
H7	0.1076	1.0810	0.1268	0.071*
C8	0.1848 (4)	1.1774 (12)	0.2322 (11)	0.070 (3)
H8	0.1906	1.2312	0.1658	0.084*
C9	0.2256 (4)	1.1893 (13)	0.3517 (13)	0.080 (4)
H9	0.2598	1.2489	0.3671	0.097*
C10	0.2165 (4)	1.1132 (16)	0.4498 (10)	0.082 (3)
H10	0.2443	1.1231	0.5319	0.098*
C11	0.1657 (4)	1.0207 (11)	0.4267 (9)	0.066 (3)
H11	0.1591	0.9707	0.4932	0.079*
C12	−0.1162 (3)	0.3945 (14)	0.1112 (8)	0.071 (3)
H12A	−0.1071	0.3243	0.0511	0.086*
H12B	−0.1327	0.5068	0.0703	0.086*
C13	−0.1609 (3)	0.2938 (14)	0.1405 (9)	0.059 (3)
C14	−0.1898 (4)	0.3716 (15)	0.2039 (10)	0.088 (3)
H14	−0.1802	0.4871	0.2360	0.105*
C15	−0.2333 (5)	0.2800 (17)	0.2209 (11)	0.100 (4)
H15	−0.2541	0.3371	0.2601	0.120*
C16	−0.2455 (4)	0.1112 (19)	0.1818 (11)	0.094 (4)
H16	−0.2737	0.0490	0.1965	0.113*
C17	−0.2171 (4)	0.0308 (14)	0.1209 (11)	0.096 (4)
H17	−0.2265	−0.0860	0.0914	0.116*
C18	−0.1744 (4)	0.1184 (18)	0.1018 (10)	0.082 (4)
H18	−0.1542	0.0591	0.0622	0.099*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0451 (5)	0.0497 (6)	0.0583 (7)	−0.0005 (7)	0.0218 (5)	0.0036 (8)
Cl1	0.0548 (15)	0.0638 (18)	0.0719 (18)	0.0134 (12)	0.0258 (14)	0.0096 (14)
Cl2	0.064 (2)	0.052 (2)	0.044 (2)	0.000	0.0224 (17)	0.000
Cl3	0.255 (7)	0.139 (6)	0.203 (7)	0.000	0.166 (6)	0.000
N1	0.040 (4)	0.046 (5)	0.037 (5)	0.002 (3)	0.016 (4)	0.004 (4)
N2	0.054 (5)	0.062 (5)	0.044 (5)	0.006 (4)	0.018 (4)	−0.013 (4)
N3	0.047 (5)	0.065 (6)	0.055 (5)	−0.002 (4)	0.020 (4)	−0.010 (4)
C1	0.029 (4)	0.034 (6)	0.075 (6)	0.000 (4)	0.017 (4)	0.000 (5)
C2	0.055 (6)	0.053 (6)	0.052 (6)	0.005 (5)	0.012 (5)	0.000 (5)
C3	0.074 (7)	0.058 (7)	0.049 (6)	−0.004 (5)	0.028 (6)	−0.007 (5)
C4	0.078 (7)	0.050 (7)	0.067 (7)	0.002 (5)	0.039 (6)	−0.002 (6)
C5	0.062 (6)	0.052 (7)	0.062 (7)	0.009 (5)	0.031 (5)	0.006 (6)
C6	0.037 (5)	0.036 (6)	0.058 (7)	0.002 (4)	0.005 (5)	−0.004 (5)
C7	0.059 (6)	0.051 (6)	0.054 (6)	−0.005 (8)	0.009 (5)	−0.004 (7)
C8	0.078 (8)	0.056 (7)	0.074 (8)	−0.023 (6)	0.027 (7)	−0.018 (6)
C9	0.061 (7)	0.052 (7)	0.123 (11)	−0.026 (5)	0.031 (8)	−0.026 (7)
C10	0.069 (7)	0.051 (9)	0.086 (9)	−0.010 (7)	−0.009 (6)	−0.007 (7)
C11	0.077 (7)	0.053 (8)	0.054 (7)	0.005 (5)	0.013 (7)	0.000 (5)
C12	0.059 (6)	0.097 (9)	0.053 (7)	−0.016 (6)	0.018 (6)	0.002 (6)
C13	0.046 (6)	0.057 (7)	0.081 (8)	0.001 (5)	0.032 (6)	0.004 (6)
C14	0.092 (8)	0.069 (8)	0.133 (10)	0.000 (6)	0.076 (8)	−0.008 (7)
C15	0.107 (9)	0.085 (10)	0.158 (12)	0.016 (8)	0.105 (9)	0.008 (9)
C16	0.085 (7)	0.066 (10)	0.155 (11)	−0.006 (8)	0.072 (7)	0.012 (10)
C17	0.093 (9)	0.058 (10)	0.154 (12)	−0.013 (6)	0.067 (9)	−0.011 (7)
C18	0.066 (7)	0.089 (11)	0.102 (8)	0.010 (7)	0.045 (6)	0.010 (9)

Geometric parameters (Å, °)

Cu1—N2	1.999 (7)	C5—H5A	0.9700
Cu1—N3	2.035 (6)	C5—H5B	0.9700
Cu1—N1	2.055 (6)	C6—C7	1.363 (11)
Cu1—Cl1	2.254 (2)	C6—C11	1.388 (10)
Cu1—Cl2	2.658 (2)	C7—C8	1.363 (11)
Cu1—Cl3	3.798 (2)	C7—H7	0.9300
Cl2—Cu1^{i}	2.658 (2)	C8—C9	1.357 (13)
N1—C1	1.444 (9)	C8—H8	0.9300
N1—C5	1.482 (9)	C9—C10	1.370 (13)
N1—H1	0.9100	C9—H9	0.9300
N2—C2	1.437 (8)	C10—C11	1.398 (11)
N2—C3	1.483 (9)	C10—H10	0.9300
N2—H2	0.9100	C11—H11	0.9300
N3—C4	1.478 (10)	C12—C13	1.518 (10)
N3—C12	1.478 (8)	C12—H12A	0.9700
N3—H3	0.9100	C12—H12B	0.9700

C1—C2	1.547 (10)	C13—C14	1.364 (11)
C1—H1A	0.9700	C13—C18	1.379 (15)
C1—H1B	0.9700	C14—C15	1.386 (12)
C2—H2A	0.9700	C14—H14	0.9300
C2—H2B	0.9700	C15—C16	1.331 (15)
C3—C4	1.515 (9)	C15—H15	0.9300
C3—H3A	0.9700	C16—C17	1.342 (13)
C3—H3B	0.9700	C16—H16	0.9300
C4—H4A	0.9700	C17—C18	1.365 (12)
C4—H4B	0.9700	C17—H17	0.9300
C5—C6	1.508 (10)	C18—H18	0.9300
N2—Cu1—N3	84.2 (3)	N3—C4—H4A	110.1
N2—Cu1—N1	83.6 (3)	C3—C4—H4A	110.1
N3—Cu1—N1	162.2 (3)	N3—C4—H4B	110.1
N2—Cu1—Cl1	171.5 (2)	C3—C4—H4B	110.1
N3—Cu1—Cl1	95.2 (2)	H4A—C4—H4B	108.4
N1—Cu1—Cl1	94.85 (19)	N1—C5—C6	113.8 (7)
N2—Cu1—Cl2	85.18 (19)	N1—C5—H5A	108.8
N3—Cu1—Cl2	97.1 (2)	C6—C5—H5A	108.8
N1—Cu1—Cl2	94.85 (19)	N1—C5—H5B	108.8
Cl1—Cu1—Cl2	103.26 (9)	C6—C5—H5B	108.8
N2—Cu1—Cl3	79.64 (19)	H5A—C5—H5B	107.7
N3—Cu1—Cl3	72.7 (2)	C7—C6—C11	118.7 (8)
N1—Cu1—Cl3	92.3 (2)	C7—C6—C5	121.2 (8)
Cl1—Cu1—Cl3	92.12 (10)	C11—C6—C5	120.2 (9)
Cl2—Cu1—Cl3	162.39 (11)	C8—C7—C6	121.8 (8)
Cu1—Cl2—Cu1^{i}	109.79 (12)	C8—C7—H7	119.1
C1—N1—C5	113.5 (6)	C6—C7—H7	119.1
C1—N1—Cu1	107.8 (5)	C9—C8—C7	120.1 (10)
C5—N1—Cu1	112.0 (5)	C9—C8—H8	119.9
C1—N1—H1	107.8	C7—C8—H8	119.9
C5—N1—H1	107.8	C8—C9—C10	119.9 (10)
Cu1—N1—H1	107.8	C8—C9—H9	120.1
C2—N2—C3	117.9 (7)	C10—C9—H9	120.1
C2—N2—Cu1	110.9 (6)	C9—C10—C11	120.2 (9)
C3—N2—Cu1	109.3 (5)	C9—C10—H10	119.9
C2—N2—H2	106.0	C11—C10—H10	119.9
C3—N2—H2	106.0	C6—C11—C10	119.2 (9)
Cu1—N2—H2	106.0	C6—C11—H11	120.4
C4—N3—C12	112.0 (7)	C10—C11—H11	120.4
C4—N3—Cu1	109.9 (5)	N3—C12—C13	115.8 (7)
C12—N3—Cu1	116.0 (5)	N3—C12—H12A	108.3
C4—N3—H3	106.0	C13—C12—H12A	108.3
C12—N3—H3	106.0	N3—C12—H12B	108.3
Cu1—N3—H3	106.0	C13—C12—H12B	108.3
N1—C1—C2	109.4 (6)	H12A—C12—H12B	107.4
N1—C1—H1A	109.8	C14—C13—C18	117.3 (9)
C2—C1—H1A	109.8	C14—C13—C12	122.2 (10)

N1—C1—H1B	109.8	C18—C13—C12	120.5 (9)
C2—C1—H1B	109.8	C13—C14—C15	120.6 (10)
H1A—C1—H1B	108.2	C13—C14—H14	119.7
N2—C2—C1	105.9 (7)	C15—C14—H14	119.7
N2—C2—H2A	110.6	C16—C15—C14	120.6 (11)
C1—C2—H2A	110.6	C16—C15—H15	119.7
N2—C2—H2B	110.6	C14—C15—H15	119.7
C1—C2—H2B	110.6	C15—C16—C17	119.9 (11)
H2A—C2—H2B	108.7	C15—C16—H16	120.1
N2—C3—C4	108.2 (7)	C17—C16—H16	120.1
N2—C3—H3A	110.1	C16—C17—C18	120.8 (12)
C4—C3—H3A	110.1	C16—C17—H17	119.6
N2—C3—H3B	110.1	C18—C17—H17	119.6
C4—C3—H3B	110.1	C17—C18—C13	120.8 (10)
H3A—C3—H3B	108.4	C17—C18—H18	119.6
N3—C4—C3	108.2 (8)	C13—C18—H18	119.6
N2—Cu1—Cl2—Cu1^{i}	−137.1 (2)	Cu1—N1—C1—C2	−37.5 (8)
N3—Cu1—Cl2—Cu1^{i}	139.3 (2)	C3—N2—C2—C1	−167.9 (7)
N1—Cu1—Cl2—Cu1^{i}	−53.97 (18)	Cu1—N2—C2—C1	−40.9 (7)
Cl1—Cu1—Cl2—Cu1^{i}	42.18 (6)	N1—C1—C2—N2	52.2 (8)
Cl3—Cu1—Cl2—Cu1^{i}	−167.59 (13)	C2—N2—C3—C4	168.9 (7)
N2—Cu1—N1—C1	12.1 (5)	Cu1—N2—C3—C4	41.1 (8)
N3—Cu1—N1—C1	59.5 (12)	C12—N3—C4—C3	164.4 (6)
Cl1—Cu1—N1—C1	−176.2 (5)	Cu1—N3—C4—C3	33.8 (8)
Cl2—Cu1—N1—C1	−72.5 (5)	N2—C3—C4—N3	−49.2 (9)
Cl3—Cu1—N1—C1	91.4 (5)	C1—N1—C5—C6	53.1 (10)
N2—Cu1—N1—C5	−113.5 (5)	Cu1—N1—C5—C6	175.6 (6)
N3—Cu1—N1—C5	−66.1 (11)	N1—C5—C6—C7	70.4 (11)
Cl1—Cu1—N1—C5	58.2 (5)	N1—C5—C6—C11	−110.6 (8)
Cl2—Cu1—N1—C5	161.9 (5)	C11—C6—C7—C8	2.9 (14)
Cl3—Cu1—N1—C5	−34.2 (5)	C5—C6—C7—C8	−178.1 (8)
N3—Cu1—N2—C2	−149.5 (6)	C6—C7—C8—C9	−0.7 (15)
N1—Cu1—N2—C2	17.4 (5)	C7—C8—C9—C10	−1.4 (15)
Cl2—Cu1—N2—C2	112.9 (5)	C8—C9—C10—C11	1.1 (16)
Cl3—Cu1—N2—C2	−76.1 (5)	C7—C6—C11—C10	−3.1 (12)
N3—Cu1—N2—C3	−17.9 (5)	C5—C6—C11—C10	177.9 (8)
N1—Cu1—N2—C3	149.0 (5)	C9—C10—C11—C6	1.1 (15)
Cl2—Cu1—N2—C3	−115.6 (5)	C4—N3—C12—C13	56.4 (10)
Cl3—Cu1—N2—C3	55.5 (5)	Cu1—N3—C12—C13	−176.2 (7)
N2—Cu1—N3—C4	−9.3 (6)	N3—C12—C13—C14	70.1 (12)
N1—Cu1—N3—C4	−56.5 (12)	N3—C12—C13—C18	−110.7 (11)
Cl1—Cu1—N3—C4	179.2 (5)	C18—C13—C14—C15	−4.0 (16)
Cl2—Cu1—N3—C4	75.1 (6)	C12—C13—C14—C15	175.3 (9)
Cl3—Cu1—N3—C4	−90.2 (5)	C13—C14—C15—C16	3.7 (18)
N2—Cu1—N3—C12	−137.6 (6)	C14—C15—C16—C17	−2.6 (19)
N1—Cu1—N3—C12	175.1 (8)	C15—C16—C17—C18	1.9 (19)
Cl1—Cu1—N3—C12	50.9 (6)	C16—C17—C18—C13	−2.4 (17)
Cl2—Cu1—N3—C12	−53.2 (6)	C14—C13—C18—C17	3.4 (16)

Cl3—Cu1—N3—C12	141.5 (6)	C12—C13—C18—C17	−175.9 (9)
C5—N1—C1—C2	87.2 (8)		

Symmetry codes: (i) −*x*, *y*, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3A···Cl3	0.97	2.82	3.640 (11)	143
C2—H2A···Cg1^{ii}	0.97	2.74	3.547 (9)	141
C15—H15···Cg1^{iii}	0.93	2.97	3.872 (14)	163

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

Fig. 1

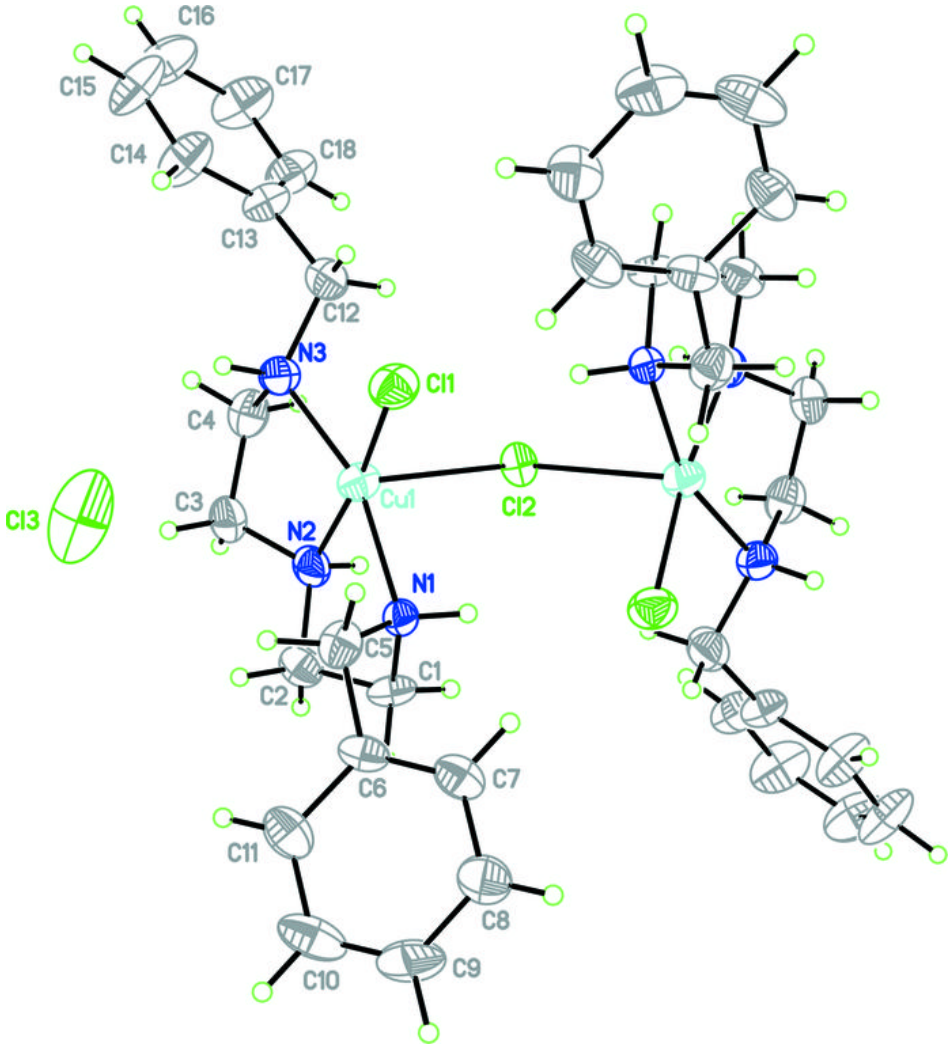
C16
C15
C17
C14
C18
C13
C12
N3
Cl1
C4
Cl3
C3
Cu1
Cl2
N2
N1
C5
C1
C2
C6
C7
C11
C8
C10
C9

Fig. 2

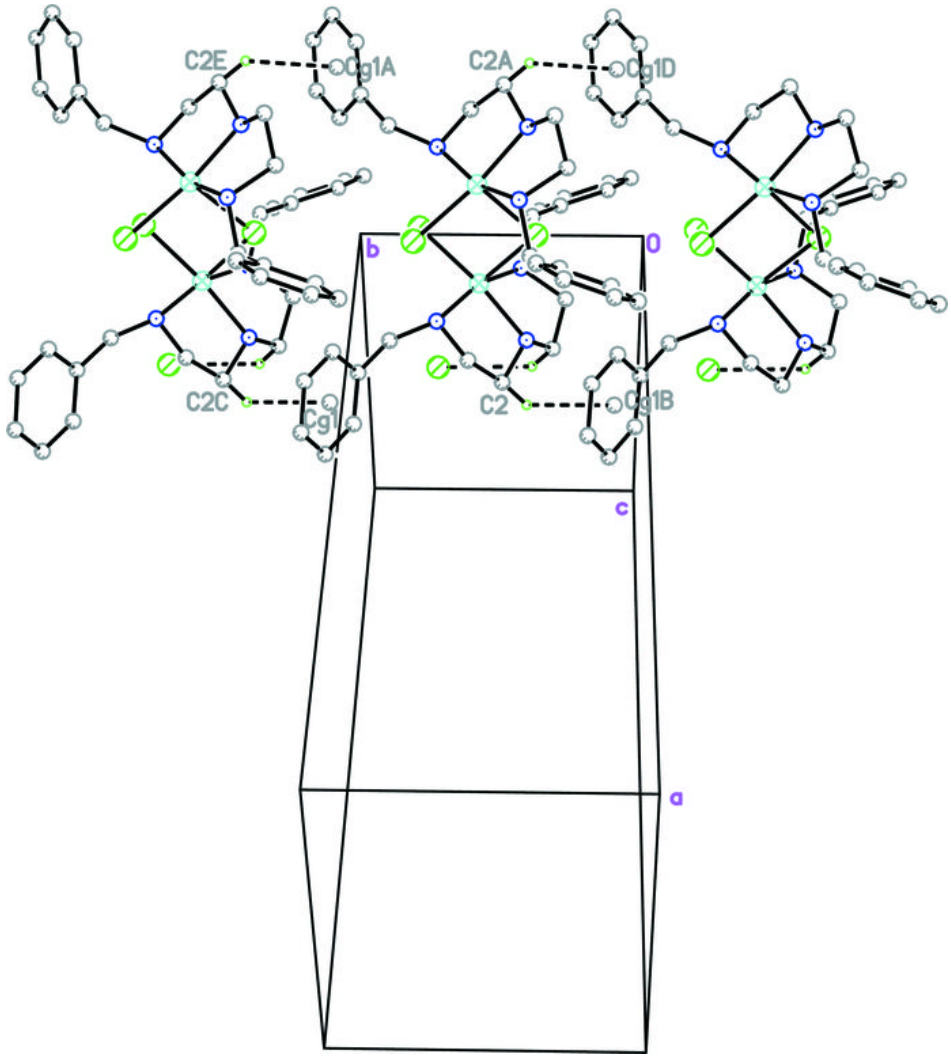

Fig. 3

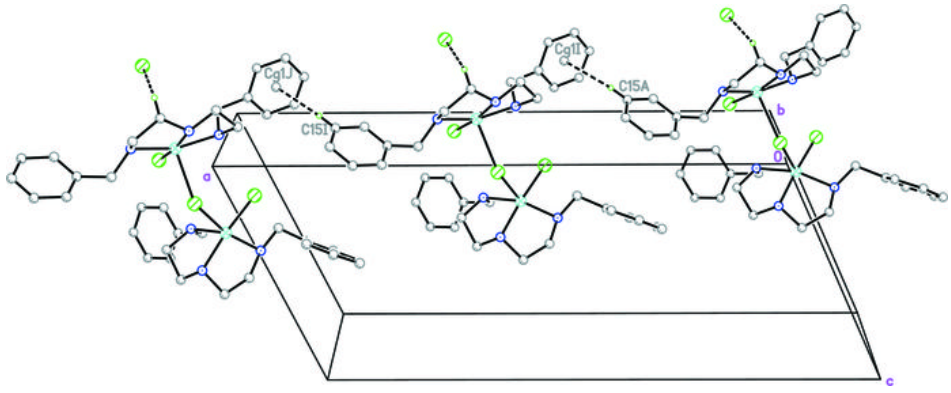

Fig. 4