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Crystal structure of *catena*-poly[[chlorido(4,4′-dimethyl-2,2′-bipyridine-$\kappa^2 N,N'$)copper(II)]-μ-chlorido]

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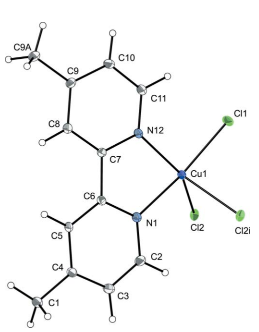
The title compound, $[CuCl_2(C_{12}H_{12}N_2)]_n$, was obtained *via* a DMSO-mediated dehydration of Cu(4,4′-dimethyl-2,2′-bipyridine)copper(II)·$0.25H_2O$. The central Cu^{II} atom is coordinated in a distorted trigonal–bipyramidal geometry by two N atoms of a chelating 4,4′-dimethyl-2,2′-bipyridine ligand [average Cu—N = 2.03 (3) Å] and three Cl atoms, one terminal with a short Cu—Cl bond of 2.2506 (10) Å, and two symmetry-equivalent and bridging bonds. The bridging Cl atom links the Cu^{II} ions into chains parallel to [001] *via* one medium and one long Cu—Cl bond [2.3320 (10) and 2.5623 (9) Å]. The structure displays both inter- and intramolecular C—H···Cl hydrogen bonding.

1. Chemical context

Bipyridine complexes of copper(II), [(2,2′-bipy)CuX_2] (X = Cl, Br) have been used in a number of important applications in recent years, most notably in the areas of catalysis for organic synthesis (Ricardo *et al.*, 2008; Csonka *et al.*, 2008; Thorpe *et al.*, 2012), DNA cleavage (Jaividhya *et al.*, 2012), degradation of pesticides (Knight *et al.*, 2014) and water oxidation (Barnett *et al.*, 2012). Such complexes are characterized by an extensive number of metal coordination geometries including square-planar/tetrahedral, square-pyramidal/trigonal–bipyramidal and distorted octahedral. The associated halide ligands (chloride, bromide) can adopt terminal or bridging bonding modes leading to monomeric, dimeric or polymeric chain structures which can influence complex solubility in organic solvents and consequently their possible application in homogeneous catalysis. A third factor which influences the structural forms of these complexes is the nature of the solvent, with strongly coordinating ligands forming solvent adducts. For example, the reaction of dimethyl-2,2′-bipyridine with Cu^I and/or Cu^{II} in DMSO or water led to the isolation of 10 different crystalline materials, suggesting that a large number of structural motifs are possible including five-coordinate monomers, distorted tetrahedral monomers, stacked planar monomers, stacked planar bibridged dimers and and five-coordinate bibridged dimers (Willett *et al.*, 2001). A large number of ring-substituted 2,2′-bipyridine complexes have also been prepared and characterized including dichlorido(4,4′-dimethyl-2,2′-bipyridine)copper(II) hemihydate. In this paper we describe the synthesis and structural characterization of a previously unknown form of dichlorido(4,4′-dimethyl-2,2′-bipyridine)copper(II) *via* a DMSO-mediated dehydration of Cu(4,4′-dimethyl-2,2′-bipyridine)Cl_2·$0.25H_2O$. The crystal structure reveals single



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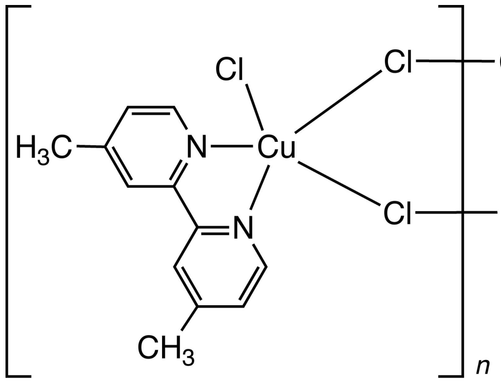
chlorido-bridged copper(II) chains with a distorted trigonal–bipyramidal geometry of the metal cations. We conclude that the presence of the 4,4′-dimethyl substituents does not prevent the formation of a catenated structure, which was previously suggested as an explanation for the dimeric arrangement in Cu(4,4′-dimethyl-2,2′-bipyridine)Cl_2·0.5H_2O (González *et al.*, 1993).



2. Structural commentary

In the title complex (**1**), Fig. 1, the central Cu^{II} atom is coordinated by the two nitrogen atoms, N1 and N12 of the chelating 2,2′-bipyridine subunit and three chlorine atoms, one terminal (Cl1) with a short Cu—Cl bond, and two bridging chlorine atoms (Cl2), which are symmetry equivalent. The bridging chlorine ligand links Cu atoms into chains *via* one medium and one long Cu—Cl bond [2.3320 (10) and 2.5623 (9) Å]. The geometry around the Cu ion is best described as a distorted trigonal bipyramid with the coordination polyhedron defined by the two N atoms and three Cl atoms, one of which links the monomeric subunits into a chain, which contrasts with the four-coordinate square-planar geometry found in Cu(2,2′-bipyridine)Cl_2 (Wang *et al.*, 2004; Garland *et al.*, 1988). The two axial sites are occupied by N1 and Cl1 [N1—Cu1—Cl1 = 172.93 (10)°] and the basal plane contains the N12 atom, the Cl2 atom and the bridging Cl2

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

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11A···Cl1	0.95	2.61	3.211 (4)	122
C8—H8A···Cl2^{i}	0.95	2.88	3.666 (4)	140
C10—H10A···Cl1^{ii}	0.95	2.88	3.733 (4)	149

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

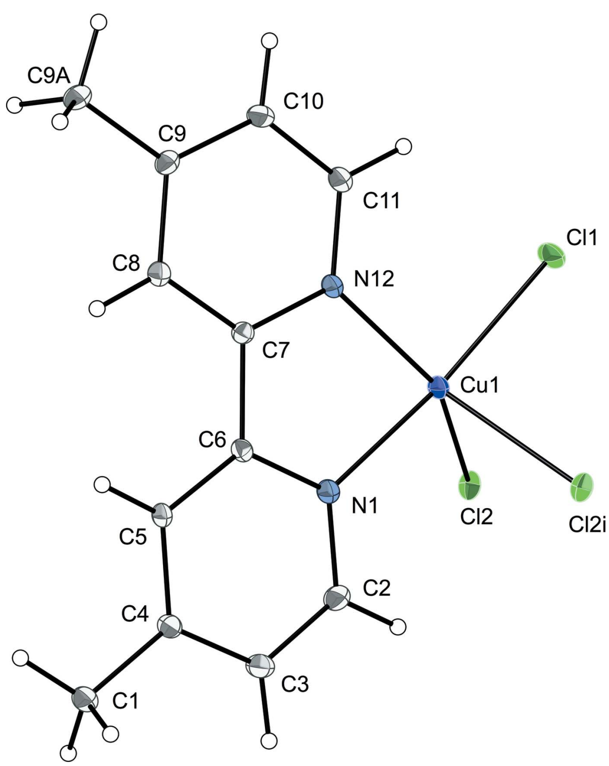


Figure 1
ORTEP-style view of compound (**1**), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: (i) $x-1, -y+2, z-\frac{1}{2}$.]

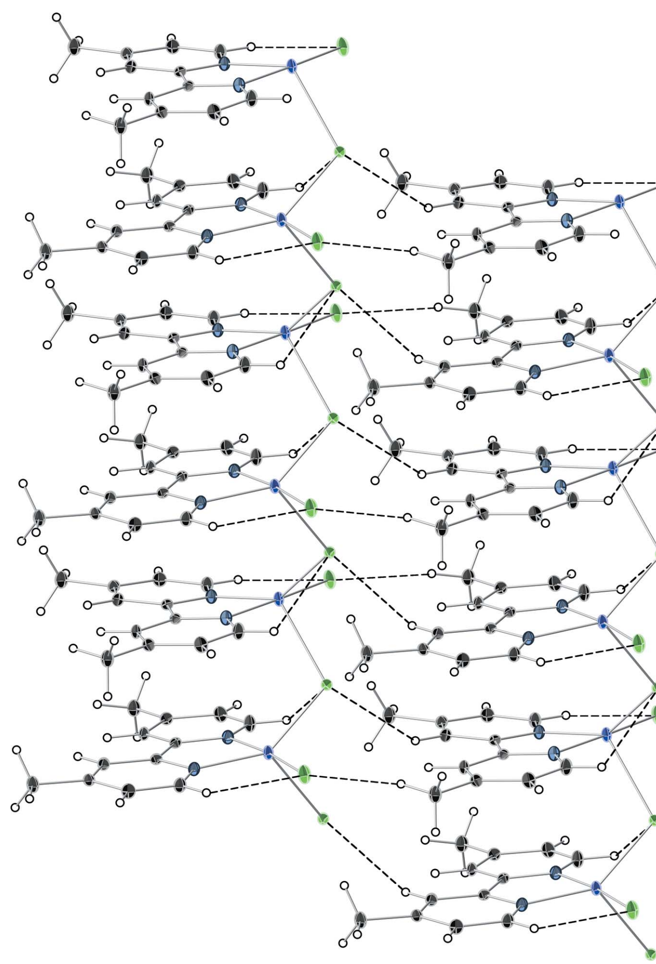


Figure 2
Selected portion of the crystal packing diagram of compound (**1**), showing interchain C—H···Cl hydrogen bonding (see Table 1 for details).

atom. The terminal Cu1—Cl1 and medium-length bridging Cu1—Cl2 bond lengths in (**1**) are 2.2506 (10) and 2.3320 (10) Å which are comparable to those found in the related structure Cu(2,2′-bipyridine)Cl_2 [2.254 (4) Å; Wang *et al.*, 2004] and its polymorph [2.291 (3) Å; Hernández-Molina *et al.*, 1999], and in dichlorido(4,4′-dimethyl)-2,2′-bipyridine)-copper(II) hemihydrate [2.255 (2) and 2.274 (2) Å, respectively; González *et al.*, 1993]. However, the longer bridging Cu—Cl bond has a length of 2.5623 (9) Å which is shorter than those found in the above comparison structures [3.047 (3), 2.674 (3) and 2.754 (2) Å]. The Cu—N1 and Cu—N12 bond lengths in (**1**) are 2.009 (3) and 2.047 (3) Å, similar to those found in the above structures [2.024 (6), 2.037 (8), and 2.001 (3) and 2.035 (4) Å, respectively]. These comparisons indicate that neither hydration nor 4,4′-dialkyl substitution significantly affects either the terminal Cu—Cl or Cu—N bond lengths. The bipyridine ring presents a bite angle of 79.25 (12)° to Cu, similar to that found in the above-mentioned structures, 80.5 (3), 79.6 (3) and 80.2 (1)° respectively, and forming a virtually planar five-membered ring. The C—C and C—N bond lengths and angles are within expected limits.

3. Supramolecular features

The crystal structure of (**1**) can best be described as a linear polymer consisting of monomeric units with chains extending parallel to [001]. The chains are connected *via* weak C—H···Cl hydrogen bonds (Table 1 and Fig. 2). Adjacent copper atoms are bridged *via* single chlorine atoms [Cu1—Cl2^{i} = 2.5623 (9) Å; (i) = $x, -y + 2, z - \frac{1}{2}$). This contrasts with the structure found in Cu(2,2′-bipyridine)Cl_2 in which two chlorine atoms link the monomeric substructures into a catenated complex. In (**1**) an intramolecular C—H···Cl hydrogen bond is also observed (Table 1).

4. Database survey

A large number of unsubstituted and substituted bipyridine copper complexes with halide ligands can be found in the Cambridge Structural Database (CSD, Version 5.35; Groom & Allen, 2015). These structures have four-, five, and six-coordination. The related structure dichlorido(4,4′-dimethyl)-2,2′-bipyridine)copper(II) hemihydrate (González *et al.*, 1993) crystallizes with a dimeric arrangement of subunits. The unsubstituted complex Cu(2,2′-bipyridine)Cl_2 has been found to form both simple monomeric (Kostakis *et al.*, 2006) and chain structures (Hernández-Molina *et al.*, 1999; Wang *et al.*, 2004), the latter bearing similarities to the structure of (**1**).

5. Synthesis and crystallization

Solvents and reagents were obtained and purified as follows: DMSO (Aldrich), dried over 4 Å molecular sieves, $CuCl_2\cdot 2H_2O$, 4,4′-dimethyl-2,2′-bipyridine (Sigma–Aldrich) used as received. Cu(4,4′-dimethyl-2,2′-bipyridine)$Cl_2\cdot$0.25 H_2O was prepared according to the literature procedure (Moore *et al.*, 2012). Cu(4,4′-dimethyl-2,2′-bipyridine)$Cl_2\cdot$0.25 H_2O (0.4091 g, 1.266 mmol) was dissolved in anhydrous DMSO (500 ml) and stored at 277 K for 30 months (shorter periods of time, *e.g.* 7 days, did not result in dehydration). The DMSO was then removed under a stream of N_2 and the resulting solid was further dried *in vacuo* at 313 K to give (**1**) as a green powder (0.386 g, 1.21 mmol, 96% yield). A portion of (**1**) was dissolved in DMSO and concentrated under a stream of N_2 (flow rate = 12 l/min) over 7 days in an open vial to give green plates. Analysis calculated for $CuC_{12}H_{12}N_2Cl_2$: C, 45.23; H, 3.80; N, 8.79. Found: C, 44.69; H, 3.66; N, 8.20.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[CuCl_2(C_{12}H_{12}N_2)]$
M_r	318.68
Crystal system, space group	Monoclinic, *Cc*
Temperature (K)	150
a, b, c (Å)	9.1101 (6), 20.0087 (12), 7.1231 (4)
β (°)	110.491 (2)
V (Å^3)	1216.25 (13)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	2.21
Crystal size (mm)	0.27 × 0.12 × 0.07
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2002)
T_{min}, T_{max}	0.646, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7099, 2945, 2829
R_{int}	0.049
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.685
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.030, 0.072, 1.05
No. of reflections	2945
No. of parameters	156
No. of restraints	2
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.56, −0.48
Absolute structure	Classical Flack method preferred over Parsons because s.u. lower (Flack, 1983)
Absolute structure parameter	0.011 (15)

Computer programs: *SMART*, *SAINT* and *XPREP* (Bruker, 2002), *SHELXS97* and *SHELXTL* (Sheldrick, 2008) and *SHELXL2014* (Sheldrick, 2015).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The H atoms were included in calculated positions and refined as riding: C—H = 0.95–0.98 Å with $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H atoms and $1.2U_{eq}(C)$ for other H atoms.

Acknowledgements

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Crystal structure of *catena*-poly[[chlorido(4,4′-dimethyl-2,2′-bipyridine-κ^2N,N')copper(II)]-μ-chlorido]

Rafaela Nita, Jeffrey R. Deschamps, Scott A. Trammell and D. Andrew Knight

Computing details

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT* and *XPREP* (Bruker, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

catena-Poly[[chlorido(4,4′-dimethyl-2,2′-bipyridine-κ^2N,N')copper(II)]-μ-chlorido]

Crystal data

$[CuCl_2(C_{12}H_{12}N_2)]$
$M_r = 318.68$
Monoclinic, *Cc*
$a = 9.1101$ (6) Å
$b = 20.0087$ (12) Å
$c = 7.1231$ (4) Å
$\beta = 110.491$ (2)°
$V = 1216.25$ (13) Å^3
$Z = 4$
$F(000) = 644$
$D_x = 1.740$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4788 reflections
$\theta = 2.6$–29.1°
$\mu = 2.21$ mm^{-1}
$T = 150$ K
Plate, green
0.27 × 0.12 × 0.07 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.646$, $T_{max} = 0.746$
7099 measured reflections
2945 independent reflections
2829 reflections with $I > 2\sigma(I)$
$R_{int} = 0.049$
$\theta_{max} = 29.1°$, $\theta_{min} = 2.0°$
$h = -12 \rightarrow 12$
$k = -27 \rightarrow 27$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.072$
$S = 1.05$
2945 reflections
156 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.0425P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.56$ e Å^{-3}
$\Delta\rho_{min} = -0.48$ e Å^{-3}

Absolute structure: Classical Flack method preferred over Parsons because s.u. lower (Flack, 1983).
Absolute structure parameter: 0.011 (15)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cu1	0.99673 (5)	0.95231 (2)	0.74601 (5)	0.01585 (12)
Cl1	1.12820 (11)	0.85482 (5)	0.80882 (16)	0.0243 (2)
Cl2	1.15771 (10)	1.00184 (5)	1.04309 (13)	0.01687 (18)
N1	0.8565 (4)	1.03282 (16)	0.6685 (5)	0.0166 (6)
C2	0.9078 (5)	1.0962 (2)	0.6952 (6)	0.0217 (8)
H2A	1.0170	1.1044	0.7567	0.026*
C3	0.8073 (5)	1.14974 (19)	0.6364 (6)	0.0213 (8)
H3A	0.8479	1.1940	0.6576	0.026*
C4	0.6467 (5)	1.13963 (18)	0.5460 (6)	0.0164 (7)
C4A	0.5357 (5)	1.19727 (19)	0.4831 (7)	0.0219 (8)
H4AA	0.4287	1.1817	0.4592	0.033*
H4AB	0.5414	1.2168	0.3597	0.033*
H4AC	0.5642	1.2311	0.5892	0.033*
C5	0.5941 (5)	1.07339 (18)	0.5156 (6)	0.0155 (6)
H5A	0.4856	1.0641	0.4530	0.019*
C6	0.7009 (4)	1.02135 (18)	0.5771 (5)	0.0136 (6)
C7	0.6593 (4)	0.94980 (17)	0.5520 (5)	0.0137 (7)
C8	0.5058 (4)	0.9266 (2)	0.4740 (6)	0.0167 (7)
H8A	0.4208	0.9573	0.4344	0.020*
C9	0.4773 (5)	0.85789 (19)	0.4542 (6)	0.0162 (7)
C9A	0.3132 (5)	0.8319 (2)	0.3748 (7)	0.0225 (8)
H9AA	0.2582	0.8514	0.2425	0.034*
H9AB	0.2588	0.8441	0.4666	0.034*
H9AC	0.3151	0.7832	0.3630	0.034*
C10	0.6064 (5)	0.81541 (19)	0.5120 (6)	0.0192 (7)
H10A	0.5919	0.7684	0.4982	0.023*
C11	0.7558 (5)	0.84178 (19)	0.5896 (6)	0.0191 (7)
H11A	0.8425	0.8120	0.6290	0.023*
N12	0.7834 (3)	0.90766 (15)	0.6114 (5)	0.0153 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.01070 (19)	0.0139 (2)	0.0205 (2)	0.00155 (17)	0.00239 (16)	0.00001 (18)
Cl1	0.0162 (4)	0.0162 (4)	0.0347 (5)	0.0053 (3)	0.0016 (4)	0.0024 (4)

Cl2	0.0135 (4)	0.0235 (4)	0.0134 (4)	−0.0012 (3)	0.0044 (3)	−0.0025 (3)
N1	0.0131 (15)	0.0153 (14)	0.0203 (15)	0.0005 (12)	0.0046 (13)	−0.0014 (12)
C2	0.0144 (18)	0.0188 (18)	0.029 (2)	−0.0023 (14)	0.0042 (16)	−0.0002 (15)
C3	0.0200 (19)	0.0150 (17)	0.026 (2)	−0.0012 (14)	0.0050 (17)	−0.0016 (15)
C4	0.0171 (17)	0.0148 (17)	0.0170 (17)	0.0004 (13)	0.0057 (14)	−0.0009 (13)
C4A	0.0179 (18)	0.0161 (18)	0.030 (2)	0.0021 (15)	0.0061 (16)	−0.0006 (16)
C5	0.0107 (15)	0.0151 (16)	0.0198 (18)	0.0020 (14)	0.0043 (14)	−0.0005 (14)
C6	0.0143 (16)	0.0144 (16)	0.0133 (16)	0.0018 (13)	0.0063 (13)	0.0007 (13)
C7	0.0149 (17)	0.0130 (16)	0.0140 (17)	0.0000 (13)	0.0062 (15)	−0.0001 (12)
C8	0.0148 (19)	0.0168 (18)	0.0184 (17)	0.0005 (13)	0.0057 (15)	−0.0008 (14)
C9	0.0154 (17)	0.0172 (17)	0.0161 (17)	−0.0030 (13)	0.0057 (14)	−0.0018 (14)
C9A	0.017 (2)	0.0190 (19)	0.029 (2)	−0.0051 (15)	0.0047 (17)	−0.0032 (16)
C10	0.0202 (18)	0.0128 (16)	0.0239 (19)	0.0004 (14)	0.0069 (16)	0.0013 (14)
C11	0.0161 (18)	0.0154 (17)	0.025 (2)	0.0028 (13)	0.0062 (16)	−0.0002 (14)
N12	0.0123 (14)	0.0136 (14)	0.0191 (15)	0.0022 (12)	0.0044 (12)	0.0000 (12)

Geometric parameters (Å, º)

Cu1—N1	2.009 (3)	C5—C6	1.387 (5)
Cu1—N12	2.047 (3)	C5—H5A	0.9500
Cu1—Cl1	2.2506 (10)	C6—C7	1.476 (5)
Cu1—Cl2	2.3320 (10)	C7—N12	1.354 (4)
Cu1—Cl2^{i}	2.5623 (9)	C7—C8	1.391 (5)
Cl2—Cu1^{ii}	2.5623 (9)	C8—C9	1.398 (5)
N1—C2	1.343 (5)	C8—H8A	0.9500
N1—C6	1.357 (5)	C9—C10	1.391 (5)
C2—C3	1.375 (6)	C9—C9A	1.494 (5)
C2—H2A	0.9500	C9A—H9AA	0.9800
C3—C4	1.392 (5)	C9A—H9AB	0.9800
C3—H3A	0.9500	C9A—H9AC	0.9800
C4—C5	1.400 (5)	C10—C11	1.382 (6)
C4—C4A	1.495 (5)	C10—H10A	0.9500
C4A—H4AA	0.9800	C11—N12	1.341 (5)
C4A—H4AB	0.9800	C11—H11A	0.9500
C4A—H4AC	0.9800		
N1—Cu1—N12	79.25 (12)	C6—C5—H5A	120.1
N1—Cu1—Cl1	172.93 (10)	C4—C5—H5A	120.1
N12—Cu1—Cl1	93.82 (9)	N1—C6—C5	121.6 (4)
N1—Cu1—Cl2	92.64 (10)	N1—C6—C7	113.8 (3)
N12—Cu1—Cl2	143.41 (9)	C5—C6—C7	124.6 (4)
Cl1—Cu1—Cl2	93.79 (4)	N12—C7—C8	122.0 (3)
N1—Cu1—Cl2^{i}	89.55 (9)	N12—C7—C6	114.5 (3)
N12—Cu1—Cl2^{i}	121.94 (9)	C8—C7—C6	123.4 (3)
Cl1—Cu1—Cl2^{i}	93.01 (4)	C7—C8—C9	119.5 (4)
Cl2—Cu1—Cl2^{i}	93.29 (3)	C7—C8—H8A	120.2
Cu1—Cl2—Cu1^{ii}	111.20 (4)	C9—C8—H8A	120.2
C2—N1—C6	118.8 (3)	C10—C9—C8	117.6 (4)

C2—N1—Cu1	124.2 (3)	C10—C9—C9A	122.0 (4)
C6—N1—Cu1	117.0 (2)	C8—C9—C9A	120.4 (4)
N1—C2—C3	122.1 (4)	C9—C9A—H9AA	109.5
N1—C2—H2A	119.0	C9—C9A—H9AB	109.5
C3—C2—H2A	119.0	H9AA—C9A—H9AB	109.5
C2—C3—C4	120.5 (3)	C9—C9A—H9AC	109.5
C2—C3—H3A	119.7	H9AA—C9A—H9AC	109.5
C4—C3—H3A	119.7	H9AB—C9A—H9AC	109.5
C3—C4—C5	117.2 (3)	C11—C10—C9	119.8 (3)
C3—C4—C4A	121.2 (3)	C11—C10—H10A	120.1
C5—C4—C4A	121.7 (4)	C9—C10—H10A	120.1
C4—C4A—H4AA	109.5	N12—C11—C10	122.7 (3)
C4—C4A—H4AB	109.5	N12—C11—H11A	118.6
H4AA—C4A—H4AB	109.5	C10—C11—H11A	118.6
C4—C4A—H4AC	109.5	C11—N12—C7	118.3 (3)
H4AA—C4A—H4AC	109.5	C11—N12—Cu1	126.3 (3)
H4AB—C4A—H4AC	109.5	C7—N12—Cu1	115.3 (2)
C6—C5—C4	119.9 (4)		

C6—N1—C2—C3	1.2 (6)	N1—C6—C7—C8	175.7 (3)
Cu1—N1—C2—C3	178.8 (3)	C5—C6—C7—C8	−4.1 (6)
N1—C2—C3—C4	0.1 (6)	N12—C7—C8—C9	−0.5 (6)
C2—C3—C4—C5	−1.0 (6)	C6—C7—C8—C9	179.5 (3)
C2—C3—C4—C4A	179.3 (4)	C7—C8—C9—C10	−0.9 (6)
C3—C4—C5—C6	0.7 (5)	C7—C8—C9—C9A	178.7 (3)
C4A—C4—C5—C6	−179.7 (4)	C8—C9—C10—C11	1.3 (6)
C2—N1—C6—C5	−1.6 (5)	C9A—C9—C10—C11	−178.3 (4)
Cu1—N1—C6—C5	−179.3 (3)	C9—C10—C11—N12	−0.4 (6)
C2—N1—C6—C7	178.6 (3)	C10—C11—N12—C7	−1.0 (6)
Cu1—N1—C6—C7	0.9 (4)	C10—C11—N12—Cu1	174.3 (3)
C4—C5—C6—N1	0.6 (6)	C8—C7—N12—C11	1.4 (6)
C4—C5—C6—C7	−179.7 (3)	C6—C7—N12—C11	−178.6 (3)
N1—C6—C7—N12	−4.3 (4)	C8—C7—N12—Cu1	−174.4 (3)
C5—C6—C7—N12	176.0 (4)	C6—C7—N12—Cu1	5.6 (4)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11*A*···Cl1	0.95	2.61	3.211 (4)	122
C8—H8*A*···Cl2^{iii}	0.95	2.88	3.666 (4)	140
C10—H10*A*···Cl1^{iv}	0.95	2.88	3.733 (4)	149

Symmetry codes: (iii) $x-1, -y+2, z-1/2$; (iv) $x-1/2, -y+3/2, z-1/2$.