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Di-μ-chloro-bis[(2,2-bipyridine)chlorocopper(II)]

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.015 Å
R factor = 0.063
wR factor = 0.180
Data-to-parameter ratio = 12.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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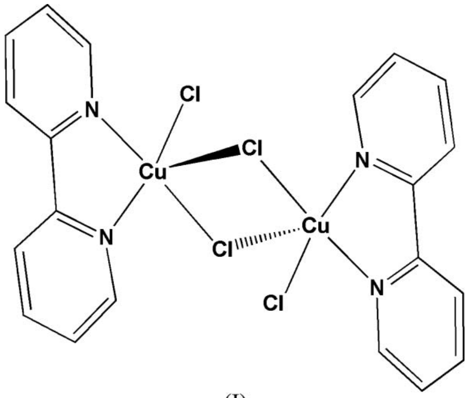
The title compound, [$Cu_2Cl_4(C_{10}H_8N_2)_2$], represents the first example of a simple dimeric coordination complex of Cu^{II} and 2,2′-bipyridine (bpy). The metal is in a five-coordinate distorted square-pyramidal environment, bonded to a 2,2′-bipyridine molecule, two bridging chlorides and one terminal chloride. There is a centre of symmetry at the mid-point of the Cu$\cdots$Cu vector.

Comment

Copper compounds display a variety of coordination geometries and coordination numbers that vary from three to six. Jahn–Teller distortion leads to the absence of regular octahedral structures in Cu^{II} chemistry. Complexes of the general formula Cu(NN)X_2 (X = Cl and/or Br; NN = a dinitrogen chelate) are known to have different geometries with the coordination number of the copper atom varying from four to six. Particular attention has been devoted to polymeric Cu^{II} complexes with chlorides and substituted bipyridines as ligands (Garland *et al.*, 1988; Hernandez-Molina *et al.*, 1999; Wang *et al.*, 2004).



(I)

The title compound, (I), represents the first example of a binuclear complex of Cu^{II} chloride and 2,2′-bipyridine and is the most distorted when compared with the other two dimeric complexes containing copper and (a substituted) bipyridine (González *et al.*, 1993; Tynan *et al.*, 2005), since the distance of the bridging chloride to a vicinal Cu atom is 2.909 (3) Å. The Cu^{II} atom is five-coordinate and the geometry about the Cu atom is square pyramidal. The coordination sites are occupied by two N atoms provided by the chelate 2,2′-bipyridine, as well as two asymmetrically bridging and one terminal chlorides. There is a centre of symmetry at the mid-point of the Cu$\cdots$Cu vector.

The interaction Cu1$\cdots$Cl1^{ii}, to form a chain structure, is very weak since the distance is 3.130 (3) Å (Wang *et al.*, 2004)

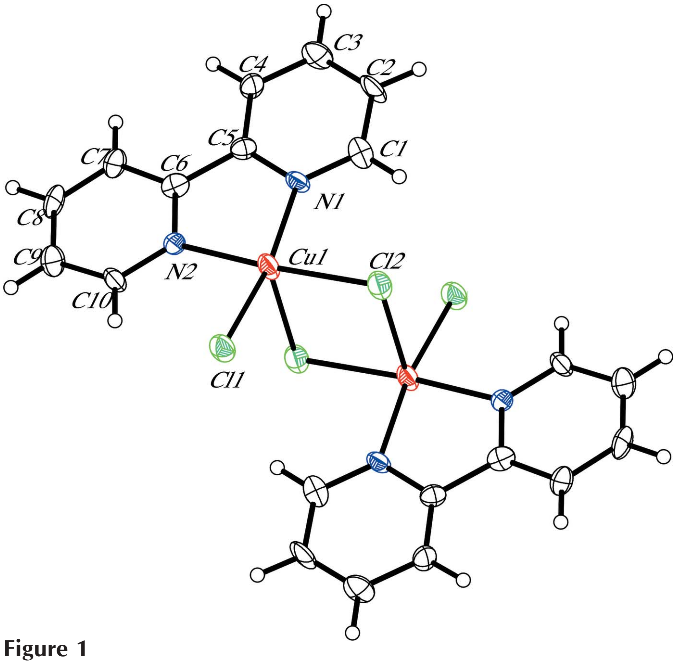


Figure 1
The molecular structure of (I), showing 40% probability displacement ellipsoids. Unlabelled atoms are related to labelled atoms by the symmetry operation $(2 - x, -y, 1 - y)$.

[symmetry code: (ii) $1 - x, -y, 1 - z$]. Although there are no stacking interactions in the crystal structure, it is stabilized by a series of intra- and inter-chain C—H···Cl contacts (Table 2 and Fig. 2). The H1—Cl2 and H10—Cl1 interactions constitute the intrachain contacts, and the H4—Cl2^{iii} and H7—Cl1^{iii} interactions are very weak inter-chain contacts [symmetry code: (iii) $x, 1 + y, z$].

Experimental

Compound (I) was produced unexpectedly. A solution of 2,2′-bipyridine (15.6 mg, 0.1 mmol) in methanol (1 ml) was added to an aqueous solution (9 ml) of $CuCl_2$ (13.3 mg, 0.1 mmol) containing an equivalent amount of *trans*-aconitic acid (11.6 mg, 0.066 mmol). A clear green solution was obtained. Green needles of (I) precipitated after slow evaporation of the solution (yield 10 mg, 35%).

Crystal data

$[Cu_2Cl_4(C_{10}H_8Cl_2N_2)_2]$
$M_r = 581.24$
Triclinic, $P\overline{1}$
$a = 7.1923$ (7) Å
$b = 8.9872$ (8) Å
$c = 9.4241$ (9) Å
$\alpha = 115.136$ (6)°
$\beta = 107.201$ (5)°
$\gamma = 95.617$ (4)°
$V = 508.91$ (8) Å^3
$Z = 1$
$D_x = 1.897$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6682 reflections
$\theta = 2.6$–24.7°
$\mu = 2.63$ mm^{-1}
$T = 120$ (2) K
Needle, green
0.22 × 0.06 × 0.02 mm

Data collection

Nonius KappaCCD diffractometer
φ scans and ω scans with κ offsets
Absorption correction: multi-scan (*XPREP* in *SHELXTL*; Sheldrick, 2005)
$T_{min} = 0.600$, $T_{max} = 0.944$
6682 measured reflections
1701 independent reflections
1142 reflections with $I > 2\sigma(I)$
$R_{int} = 0.103$
$\theta_{max} = 24.7°$
$h = -8 \rightarrow 8$
$k = -10 \rightarrow 10$
$l = -10 \rightarrow 11$

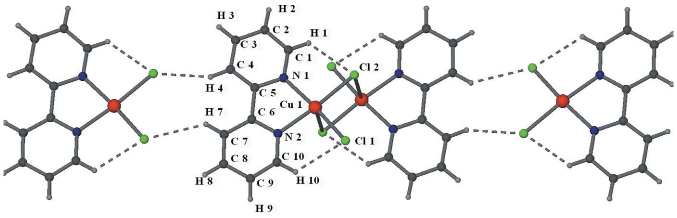


Figure 2
A representation of intra- and inter-chain C—H···Cl contacts (dashed lines), resulting in the formation of a one-dimensional chain.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.063$
$wR(F^2) = 0.180$
$S = 1.17$
1701 reflections
136 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.066P)^2 + 2.6959P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.09$ e Å^{-3}
$\Delta\rho_{min} = -0.84$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N2	2.024 (7)	Cu1—Cl2	2.280 (3)
Cu1—N1	2.037 (7)	Cu1—Cl2^{i}	2.909 (3)
Cu1—Cl1	2.272 (3)	Cl1—Cu1^{ii}	3.130 (3)
N2—Cu1—N1	81.0 (3)	Cl1—Cu1—Cl2	92.52 (9)
N2—Cu1—Cl1	93.4 (2)	N2—Cu1—Cl2^{i}	88.4 (2)
N1—Cu1—Cl1	170.2 (2)	N1—Cu1—Cl2^{i}	90.1 (2)
N2—Cu1—Cl2	174.0 (2)	Cl1—Cu1—Cl2^{i}	97.79 (9)
N1—Cu1—Cl2	93.3 (2)	Cl2—Cu1—Cl2^{i}	89.91 (8)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···Cl2	0.95	2.61	3.209 (11)	121
C10—H10···Cl1	0.95	2.62	3.209 (9)	121
C7—H7···Cl1^{iii}	0.95	2.81	3.542 (10)	135
C4—H4···Cl2^{iii}	0.95	2.69	3.517 (10)	146

Symmetry code: (iii) $x, y + 1, z$.

The H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.95 Å and $U_{iso}(H) = 1.2U_{eq}$(parent atom). The highest density peak is loacted 1.09 Å from atom Cu1.

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *DENZO*/*SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO*/*SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Crystal Impact, 2005) and *X-SEED* (Barbour, 2001); software used to prepare material for publication: *SHELXL97*.

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