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Di-μ-chloro-bis[chloro(dipyridophenazine-κ^2N,N')copper(II)]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.011 Å
R factor = 0.051
wR factor = 0.137
Data-to-parameter ratio = 13.5

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

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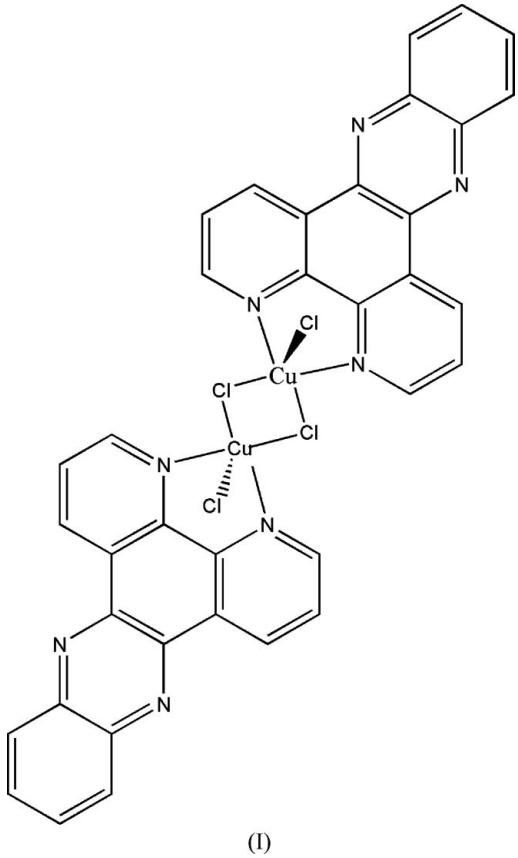
The title compound, $[Cu_2Cl_4(C_{18}H_{10}N_4)_2]$, has a discrete binuclear structure, in which the Cu atoms show square-pyramidal geometry. The complex molecule is centrosymmetric. There are strong intermolecular π–π stacking interactions between the dipyridophenazine ligands.

Comment

Dipyridophenazine derivatives are usually used as molecular light switches (Hartshorn & Barton, 1992) for the study of fast electron transfer through DNA (Murphy *et al.*, 1993). A ruthenium(II) complex with dipyridophenazine has been found to be a good cleavage agent with high affinity for DNA (Gupta *et al.*, 1992). We report here the synthesis and structure of the title binuclear copper(II) complex of dipyridophenazine, (I).



(I)

Complex (I) has a discrete binuclear structure lying on a centre of symmetry (Fig. 1 and Table 1). The asymmetric unit contains one dipyridophenazine ligand, two Cl atoms and one Cu atom. Planar dipyridophenazine ligands from adjacent

binuclear molecules at (x, y, z) and $(-x+1, -y, -z+2)$ are paired to furnish strong π–π stacking interactions, with an average plane-to-plane separation of 3.20 Å (Zheng *et al.*, 2001).

Experimental

A mixture of $CuCl_2{\cdot}2H_2O$ (0.085 g, 0.5 mmol), dipyridophenazine (0.141 g, 0.5 mmol) and water (10 ml) was sealed in a 23 ml Teflon-lined reactor and heated at 453 K for 6 d, and then cooled to room temperature at a rate of 5 K h^{-1} (yield 30%). Analysis, calculated for $C_{36}H_{20}Cl_4Cu_2N_8$: C 51.88, H 2.42, N 13.44%; found: C 51.56, H 2.25, N 13.73%.

Crystal data

$[Cu_2Cl_4(C_{18}H_{10}N_4)_2]$	V = 794.37 (17) Å^3
M_r = 833.48	Z = 1
Triclinic, $P\overline{1}$	D_x = 1.742 Mg m^{-3}
a = 7.2207 (9) Å	Mo $K\alpha$ radiation
b = 7.9232 (10) Å	μ = 1.72 mm^{-1}
c = 14.6183 (18) Å	T = 293 (2) K
α = 98.360 (2)°	Block, green
β = 101.476 (2)°	0.37 × 0.21 × 0.12 mm
γ = 99.546 (2)°	

Data collection

Bruker SMART APEX area-detector diffractometer	4386 measured reflections
	3062 independent reflections
φ and ω scans	2617 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	R_{int} = 0.020
	θ_{max} = 26.0°
T_{min} = 0.570, T_{max} = 0.816	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0719P)^2 + 0.7132P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.051	
$wR(F^2)$ = 0.137	
S = 1.06	$(\Delta/\sigma)_{max} < 0.001$
3062 reflections	$\Delta\rho_{max}$ = 0.79 e Å^{-3}
226 parameters	$\Delta\rho_{min}$ = −0.47 e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Cu1—N2	2.026 (5)	Cu1—Cl2	2.2787 (17)
Cu1—N1	2.042 (6)	Cu1—Cl2^{i}	2.7582 (19)
Cu1—Cl1	2.2394 (19)		
N2—Cu1—N1	80.3 (2)	Cl1—Cu1—Cl2	92.07 (7)
N2—Cu1—Cl1	169.97 (16)	N2—Cu1—Cl2^{i}	88.48 (16)
N1—Cu1—Cl1	93.69 (16)	N1—Cu1—Cl2^{i}	93.58 (16)
N2—Cu1—Cl2	93.25 (16)	Cl1—Cu1—Cl2^{i}	99.98 (7)
N1—Cu1—Cl2	172.35 (16)	Cl2—Cu1—Cl2^{i}	90.36 (6)

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

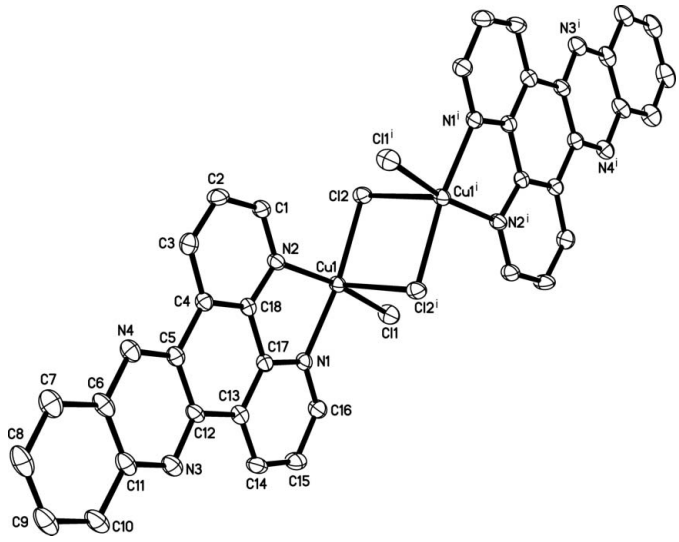


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry code: (i) $-x, -y, 1-z$.]

H atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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